Access DB# 185632

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Wayne Langel Examiner #: 60603 Date: 4-17-06
Art Unit: 1754 Phone Number ~~30~~ 2-1353 Serial Number: 10/669297
Mail Box and Bldg/Room Location: E09A29 (Remsen) Results Format Preferred (circle) PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Methods for the production of hydrogen

Inventors (please provide full names): Leonid Grigorian

Earliest Priority Filing Date: 9-26-02

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search claims 1-24 as attached hereto. Note that the invention lies in including iodine with the hydrocarbon fuel.

SCIENTIFIC REFERENCE BR
Sci & Tech Inf. Cntr
APR 17 REC'D
Pat. & T.M. Office

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STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: EJ	NA Sequence (#)	STN
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#)	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed: 4-26-06	Litigation	Lexis/Nexis
Searcher Prep & Review Time:	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time:	Other	Other (specify)

PTO-1590 (8-01)

10/669297
AU1754

We claim:

1. A method for generation of hydrogen gas, the method comprising:
contacting a hydrocarbon fuel with iodine to provide a mixture thereof; and
heating the mixture thereby generating hydrogen gas.

2. The method of claim 1, wherein the hydrocarbon fuel is a cycloalkane or an aryl compound, or mixtures thereof.

3. The method of claim 2, wherein the hydrocarbon is a cycloalkane compound.

4. The method of claim 3, wherein the cycloalkane is cyclohexane.

5. The method of claim 2, wherein the hydrocarbon is an aryl compound.

6. The method of claim 5, wherein aryl compound is benzene.

7. The method of claim 2, wherein the hydrocarbon is a mixture of a cyclohexane and an aryl compound selected from the group consisting of benzene and toluene.

8. The method of claim 1, wherein the hydrocarbon fuel and iodine are in a ratio of about 1:0.001 to about 1:2 moles/moles.

9. The method of claim 8, wherein the ratio is about 1:0.01 to about 1:0.25 moles/moles.

10. The method of claim 1, wherein the mixture is heated to a temperature of about 60°C to about 500°C.

11. The method of claim 10, wherein the mixture is heated to a temperature greater than about 80°C to about 100°C.

12. The method of claim 10, wherein the mixture is heated to a temperature greater than about 80°C.

13. The method of claim 1, further comprising exposing providing the mixture to increased pressure.

14. The method of claim 13 wherein the pressure is greater than about 1 atmosphere, and less than about 250 atmospheres.

15. The method of claim 14, wherein the pressure is greater than about 2 atmospheres.

16. A method comprising the steps of:

providing in a reaction container a composition comprising a hydrocarbon fuel and iodine; and

causing the composition to react in the container to generate hydrogen gas.

17. The method of claim 16, further comprising recovering the hydrogen gas.

18. The method of claim 17, further comprising using the recovered hydrogen gas as a fuel.

19. The method of claim 16, wherein the hydrocarbon fuel is selected from the group consisting of cyclohexane and benzene, or mixtures thereof.

20. The method of claim 19, wherein the hydrocarbon fuel is cyclohexane.

21. The method of claim 20, wherein the hydrocarbon fuel is benzene.

22. The method of claim 16, wherein the hydrocarbon fuel and iodine are in a ratio of about 1:0.001 to about 1:2 moles/moles.

23. The method of claim 22, wherein the ratio is about 1:0.01 to about 1:0.25 moles/moles.

24. The method of claim 23, wherein the ratio is about 1:0.05 to about 1:0.2 moles/moles.

25. A fuel cell system comprising:

a hydrogen gas generator of claim 16; and

a fuel cell capable of generating electricity by making use of hydrogen gas as a fuel.

26. The fuel cell of claim 25, wherein the hydrogen gas is generated by an increase in temperature and /or an increase in pressure.

27. The fuel cell of claim 26, wherein the hydrogen gas is generated by an increase in temperature and an increase in pressure.

28. The fuel cell of claim 26, wherein the hydrogen gas is generated by first increasing the temperature and then increasing the pressure.

29. The fuel cell of claim 26, wherein the hydrogen gas is generated by first increasing the pressure and then increasing the temperature.

30. The fuel cell of claim 26, wherein the temperature is increased to about 80°C or higher.

31. The fuel cell of claim 26, wherein the pressure is increased to greater than about 2 atmospheres.

32. The fuel cell of claim 26, wherein the temperature is between about 80°C and 100°C, and the pressure is between about 2 atmospheres and 2.5 atmospheres.

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=> file reg
FILE 'REGISTRY' ENTERED AT 10:21:47 ON 26 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> display history full l1-

     FILE 'REGISTRY' ENTERED AT 09:43:48 ON 26 APR 2006
                      E HYDROGEN/CN
L1                  1 SEA HYDROGEN/CN
L2             174471 SEA (C(L)H)/ELS (L) 2/ELC.SUB
                      E CYCLOHEXANE/CN
L3                  1 SEA CYCLOHEXANE/CN
                      E BENZENE/CN
L4                  1 SEA BENZENE/CN
                      E IODINE/CN
L5                  1 SEA IODINE/CN

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L6              32138 SEA (PRODUC? OR PROD# OR GENERAT? OR MANUF? OR MFR# OR
                      CREAT? OR FORM## OR FORMING# OR FORMAT? OR MAKE# OR
                      MADE# OR MAKING# OR FABRICAT? OR SYNTHESI? OR PREPAR? OR
                      PREP#)/BI,AB

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                      OR GENERAT? OR MANUF? OR MFR# OR CREAT? OR FORM## OR
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                      FABRICAT? OR SYNTHESI? OR PREPAR? OR PREP#)
L8            1457193 SEA L2
L9             291148 SEA L2 (L) RACT/RL
L10             98650 SEA L3 OR C6H12 OR CYCLOHEXANE#
L11            281493 SEA L4 OR C6H6
L12            180739 SEA L5 OR I2 OR IODINE# OR (MOLECUL? OR ELEMENT? OR
                      PURE# OR PURIF? OR REAGENT? OR REACTANT?)(A)I
L13              6761 SEA L3 (L) RACT/RL
L14             19029 SEA L4 (L) RACT/RL
L15              7634 SEA L5 (L) RACT/RL
L16               468 SEA L7 AND L8 AND L12
L17               166 SEA L16 AND L9
L18                68 SEA L16 AND L10
L19               111 SEA L16 AND L11
L20                14 SEA L16 AND L13
L21                13 SEA L16 AND L14
L22                50 SEA L16 AND L15
L23             35156 SEA L1/P
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L24             6 SEA L22 AND L23
L25            40 SEA L16 AND L23
L26            17 SEA L17 AND L23
L27             6 SEA L18 AND L23
L28             6 SEA L19 AND L23
L29            20 SEA L17 AND L18
L30            21 SEA L17 AND L19
L31            29 SEA L18 AND L19
L32          1750 SEA (HYDROCARBON# OR CYCLOHEXANE# OR C6H12 OR BENZENE#
                  OR C6H6)(3A)(I2 OR IODINE#)

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                  OR COMPOSIT? OR COMPN# OR COMPSN# OR FORMULAT? OR
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                  IMMIX? OR INTERMIX? OR DOPE# OR DOPING# OR DOPANT? OR
                  COMPOSIT? OR COMPN# OR COMPSN# OR FORMULAT? OR COMBINAT?
                  OR INTERSPER?)
L35             4 SEA L34 AND L7
L36            62 SEA L32 AND L7
L37           117 SEA L23 AND L15
L38             1 SEA L37 AND L13
L39             1 SEA L37 AND L14
L40             6 SEA L37 AND (L8 OR L9 OR L10 OR L11 OR HYDROCARBON#)

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                  E TOLUENE/CN
L41             1 SEA TOLUENE/CN

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L42        179508 SEA L41 OR MEC6H5 OR CH3C6H5 OR C6H5ME OR C6H5CH3 OR
                  TOLUENE# OR METHYLBENZENE#
L43         14441 SEA L41 (L) RACT/RL
L44          3044 SEA L7 AND L12
L45            81 SEA L44 AND L42
L46             6 SEA L44 AND L43
L47           300 SEA L7 AND L15
L48             7 SEA L47 AND L42
L49             1 SEA L47 AND L43
L50            24 SEA L24 OR L27 OR L28 OR L35 OR L38 OR L39 OR L40 OR L48
                  OR L49
L51            19 SEA (L20 OR L21 OR L26) NOT L50
L52            32 SEA (L29 OR L30 OR L31) NOT (L50 OR L51)
L53            22 SEA L25 NOT (L50 OR L51 OR L52)
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L54             33 SEA L22 NOT (L50 OR L51 OR L52 OR L53)
L55             23 SEA L50 AND (1840-2002/PRY OR 1840-2002/PY)
L56             16 SEA L51 AND (1840-2002/PRY OR 1840-2002/PY)
L57             32 SEA L52 AND (1840-2002/PRY OR 1840-2002/PY)
L58             22 SEA L53 AND (1840-2002/PRY OR 1840-2002/PY)
L59             27 SEA L54 AND (1840-2002/PRY OR 1840-2002/PY)
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=> file hca
FILE 'HCA' ENTERED AT 10:22:07 ON 26 APR 2006

=> d l55 1-23 cbib abs hitstr hitind

L55 ANSWER 1 OF 23 HCA COPYRIGHT 2006 ACS on STN

141:72799 Method to produce the halogenated polymers by electrochemical in situ generation of halogen. Khusainova, R. M.; Dorozhkin, V. P.; Shiyapov, R. T.; Khairullin, R. V.; Maksimov, D. A. (Russia). Russ. RU 2217440 C2 20031127, No pp. given (Russian). CODEN: RUXXE7. APPLICATION: RU 2000-128561 20001117.

AB Accoring to the method of the invention a comminuted polymer or its nonaq. soln. is suspended in the aq. soln. of a halogen compd. in a chem. reactor, and the halogen is generated electrochem. in situ. The method involves fewer stages, uses inexpensive starting materials and has ecol. advantages over currently used technol..

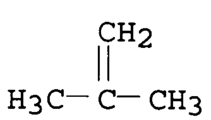
IT **9010-85-9P**
(butyl rubber, brominated; method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 9010-85-9 HCA

CN 1,3-Butadiene, 2-methyl-, polymer with 2-methyl-1-propene (9CI) (CA INDEX NAME)

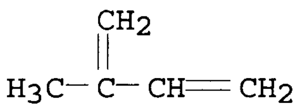
CM 1

CRN 115-11-7
CMF C4 H8



CM 2

CRN 78-79-5
CMF C5 H8



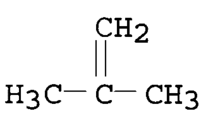
(butyl rubber, chlorinated; method to produce the halogenated polymers by electrochem. in situ generation of halogen

IT **9010-85-9**
(butyl rubber, method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 9010-85-9 HCA
CN 1,3-Butadiene, 2-methyl-, polymer with 2-methyl-1-propene (9CI) (CA INDEX NAME)

CM 1

CRN 115-11-7
CMF C4 H8



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CRN 78-79-5
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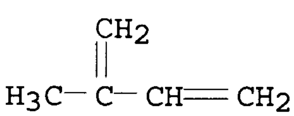


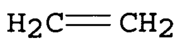
IT **9002-88-4**, Polyethylene
(high-pressure; method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 9002-88-4 HCA
CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

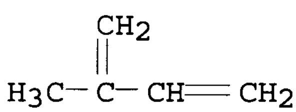
CMF C2 H4



IT **9003-31-0P**
(isoprene rubber, chlorinated; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
RN 9003-31-0 HCA
CN 1,3-Butadiene, 2-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

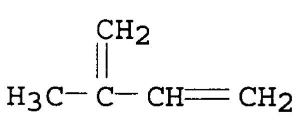
CRN 78-79-5
CMF C5 H8



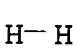
IT **9003-31-0**
(isoprene rubber, of cis-1,4-configuration; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
RN 9003-31-0 HCA
CN 1,3-Butadiene, 2-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 78-79-5
CMF C5 H8



IT **1333-74-0P, Hydrogen, preparation**
(method to produce the halogenated polymers by electrochem. in situ generation of halogen)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)



IT **9002-88-4DP**, Polyethylene, chlorinated

(method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4

$H_2C{=}CH_2$

IT **7553-56-2P, Iodine,** preparation

(method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **25034-71-3**, Ethylene-dicyclopentadiene-propylene copolymer

(rubber; method to produce the halogenated polymers by electrochem. in situ generation of halogen)

RN 25034-71-3 HCA

CN 4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro-, polymer with ethene and 1-propene (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

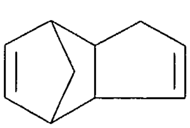
CMF C3 H6

$H_3C{-}CH{=}CH_2$

CM 2

CRN 77-73-6

CMF C10 H12



CM 3

CRN 74-85-1
CMF C2 H4

$H_2C{=}CH_2$

IC ICM C08F008-18
ICS C08F008-20; C08F008-22; C08C019-12; C08C019-14
CC 39-4 (Synthetic Elastomers and Natural Rubber)
Section cross-reference(s): 35, 72
IT **9010-85-9P**
(butyl rubber, brominated; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9010-85-9P**
(butyl rubber, chlorinated; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9010-85-9**
(butyl rubber, method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9002-88-4**, Polyethylene
(high-pressure; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9003-31-0P**
(isoprene rubber, chlorinated; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9003-31-0**
(isoprene rubber, of cis-1,4-configuration; method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **1333-74-0P, Hydrogen, preparation**
(method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **9002-88-4DP**, Polyethylene, chlorinated
(method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **7553-56-2P, Iodine**, preparation 7726-95-6P, Bromine, preparation 7782-50-5P, Chlorine, preparation
(method to produce the halogenated polymers by electrochem. in situ generation of halogen)
IT **25034-71-3**, Ethylene-dicyclopentadiene-propylene copolymer
(rubber; method to produce the halogenated polymers by electrochem. in situ generation of halogen)

L55 ANSWER 2 OF 23 HCA

140:289803 **Generation** of **hydrogen** using **iodine** as a catalyst and its use as a fuel. Grigorian, Leonid (Honda Motor Co., Ltd., Japan). PCT Int. Appl. WO 2004028961 A1 20040408, 16 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-JP12330 20030926. PRIORITY: US 2002-2002/PV41446U 20020926; US 2003-2003/PV443246 20030128.

AB **Hydrogen** is **generated** by dissolving a catalytic amt. of **iodine** in a hydrocarbon fuel source and heating the mixt. to 60-500.degree.. The hydrocarbon fuel can be a cycloalkane, preferably **cyclohexane**, or an aryl compd., preferably benzene and toluene, or their mixts. The hydrocarbon/ **iodine** ratio is 1:(0.01-0.25). The reaction mixt. is exposed to an increased pressure of > 2 atm. The hydrogen can be purified and used as fuel in a fuel cell to generate electricity.

IT **7553-56-2**, **Iodine**, uses
(**generation** of **hydrogen** using **iodine** as catalyst and its use as fuel)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **1333-74-0P**, **Hydrogen**, **preparation**
(**generation** of **hydrogen** using **iodine** as catalyst and its use as fuel)

RN 1333-74-0 HCA

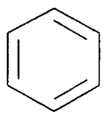
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

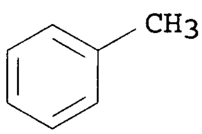
IT **71-43-2**, Benzene, reactions **108-88-3**, Toluene, reactions **110-82-7**, **Cyclohexane**, reactions **540-84-1**, Isooctane
(**generation** of **hydrogen** using **iodine** as catalyst and its use as fuel)

RN 71-43-2 HCA

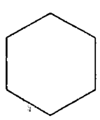
CN Benzene (8CI, 9CI) (CA INDEX NAME)



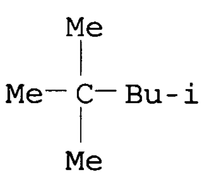
RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 540-84-1 HCA
CN Pentane, 2,2,4-trimethyl- (8CI, 9CI) (CA INDEX NAME)



IC ICM C01B003-26
ICS B01J027-00; H01M008-06
CC 51-11 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 49, 52, 67
ST **hydrogen manuf** cycloalkane aryl **iodine** catalyst fuel cell
IT Fuel cells
(**generation** of **hydrogen** using **iodine** as catalyst and its use as fuel)
IT Aromatic hydrocarbons, reactions
Cycloalkanes
(**generation** of **hydrogen** using **iodine** as catalyst and its use as fuel)
IT Power

(**generation**; **generation** of **hydrogen**
using **iodine** as catalyst and its use as fuel)

IT 7440-44-0P, Carbon, **preparation**
(**generation** of **hydrogen** using **iodine**
as catalyst and its use as fuel)

IT **7553-56-2**, **Iodine**, uses
(**generation** of **hydrogen** using **iodine**
as catalyst and its use as fuel)

IT **1333-74-0P**, **Hydrogen**, **preparation**
(**generation** of **hydrogen** using **iodine**
as catalyst and its use as fuel)

IT **71-43-2**, Benzene, reactions **108-88-3**, Toluene,
reactions **110-82-7**, **Cyclohexane**, reactions
540-84-1, Isooctane
(**generation** of **hydrogen** using **iodine**
as catalyst and its use as fuel)

L55 ANSWER 3 OF 23 HCA COPYRIGHT 2006 ACS on STN

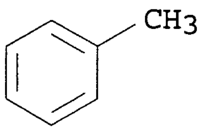
140:93671 Process for preparation of fluorine-containing alkyl halides. Katsube, Toshiyuki; Noda, Kouzou; Miki, Jun (Daikin Industries, Ltd., Japan). PCT Int. Appl. WO 2004005225 A1 20040115, 22 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2003-JP7954 20030624. PRIORITY: JP 2002-194175 20020703; JP 2002-353958 20021205.

AB This invention pertains to a method for producing fluorine-contg. alkyl halides with general formula of Rf-CH2CH2X [wherein Rf = perfluoroalkyl or polyfluoroalkyl; X = halo] which comprises reacting Rf-CH=CH2 with HX (prepd. in situ) in the presence or absence of a catalyst. For example, C8F17CH=CH2 was treated with aq. KI soln. in the presence of P2O5 and activated carbon to give C8F17CH2CH2I. According to the invention, fluorine-contg. alkyl halides can be efficiently prepd. from fluorine-contg. alkenes, and fluorine-contg. esters can be also efficiently prepd. from the alkyl halides obtained.

IT **108-88-3**, **Toluene**, uses
(prepn. of fluorine-contg. alkyl halides)

RN 108-88-3 HCA

CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **7553-56-2**, Iodine, reactions
(**prepn.** of fluorine-contg. alkyl halides)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

IC ICM C07C017-087
ICS C07C019-16; C07C019-08; C07C067-10; C07C069-653
CC 23-3 (Aliphatic Compounds)
IT **Hydrogen** halides
(**prepn.** of fluorine-contg. alkyl halides)
IT 50-32-8, Benzo[a]pyrene, uses 56-55-3, Benzanthracene 71-43-2, Benzene, uses 85-01-8, Phenanthrene, uses 91-20-3, Naphthalene, uses 92-24-0, Naphthacene 95-47-6, o-Xylene, uses 106-42-3, p-Xylene, uses 108-38-3, m-Xylene, uses **108-88-3**, **Toluene**, uses 119-64-2, 1,2,3,4-Tetrahydronaphthalene 120-12-7, Anthracene, uses 129-00-0, Pyrene, uses 447-53-0, 1,2-Dihydronaphthalene 612-17-9, 1,4-Dihydronaphthalene 7440-44-0, Carbon, uses 7487-88-9, Magnesium sulfate, uses 7757-82-6, Sodium sulfate, uses 7778-18-9, Calcium sulfate 7778-80-5, Potassium sulfate, uses 10043-01-3, Aluminum sulfate
(prepn. of fluorine-contg. alkyl halides)
IT 64-18-6, Formic acid, reactions 64-19-7, Acetic acid, reactions 79-09-4, Propionic acid, reactions 107-92-6, Butyric acid, reactions 109-52-4, Pentanoic acid, reactions 142-62-1, Hexanoic acid, reactions 1333-74-0, **Hydrogen**, reactions 7440-68-8, Astatine, reactions **7553-56-2**, Iodine, reactions 7664-38-2, Phosphoric acid, reactions 7726-95-6, Bromine, reactions 7732-18-5, Water, reactions 7782-41-4, Fluorine, reactions 7782-50-5, Chlorine, reactions 10343-62-1, Metaphosphoric acid 21652-58-4
(**prepn.** of fluorine-contg. alkyl halides)

L55 ANSWER 4 OF 23 HCA COPYRIGHT 2006 ACS on STN
139:214117 Process for preparation of optically active 3-halo-1,2-propanediol derivatives. Taoka, Naoaki; Sugawara, Masanobu; Yasohara, Yoshihiko (Kaneka Corporation, Japan). PCT Int. Appl. WO 2003070676 A1 20030828, 38 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR,

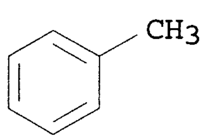
CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2003-JP1962 20030224. PRIORITY: JP 2002-45761 20020222.

AB This invention pertains to a method for producing 3-halo-1,2-propanediol derivs. from inexpensive materials. The process comprises reacting 2-chloroallyl alc., which is easily available at low cost, with a hypohalogenous acid salt or a halogen to convert the alc. into a halohydroxyacetone deriv. and subsequently asym. hydrogenation of the halohydroxyacetone deriv. with hydrogen in the presence of an asym. hydrogenation catalyst prepd. from a transition metal and an optically active phosphine ligand to produce an optically active 3-halo-1,2-propanediol deriv. For example, 2,3-dichloropropene was treated with K2CO3 in H2O, followed by the addn. of H2SO4 and aq. NaOCl to give 1-chloro-3-hydroxyacetone. The acetone was recrystd. from PhMe and hexane to produce 2,5-di(chloromethyl)-2,5-dihydroxy-1,4-dioxane. The dioxane was hydrogenated with H2 in MeOH and H2O in the presence of RuBr2(S)-BINAP to afford (R)-3-chloro-1,2-propanediol (93%).

IT **108-88-3**, **Toluene**, uses
(prepn. of optically active chloropropanediol derivs.)

RN 108-88-3 HCA

CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **7553-56-2**, Iodine, reactions
(**prepn.** of optically active chloropropanediol derivs.)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IC ICM C07C045-30
ICS C07C049-173; C07C029-145; C07C031-42; C07D319-12; C07B053-00; C07B061-00

CC 23-7 (Aliphatic Compounds)

IT 56-23-5, Carbon tetrachloride, uses 60-29-7, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0,

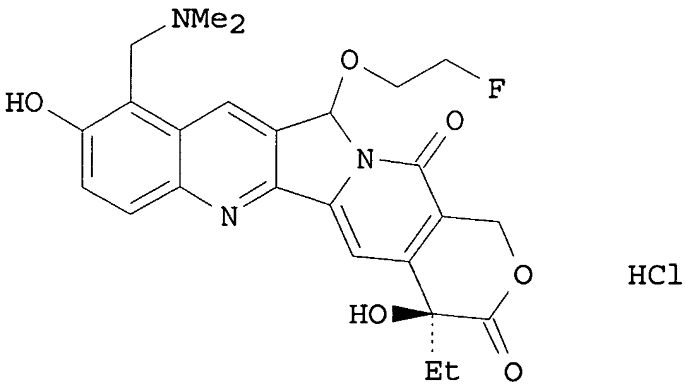
Isopropanol, uses 67-64-1, Acetone, uses 67-66-3, Chloroform, uses 71-23-8, Propanol, uses 71-36-3, 1-Butanol, uses 71-43-2, Benzene, uses 75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 78-93-3, Methyl ethyl ketone, uses 79-20-9, Methyl acetate 95-47-6, o-Xylene, uses 96-22-0, Diethyl ketone 98-82-8, Cumene 100-41-4, Ethylbenzene, uses 100-66-3, Anisole, uses 103-65-1, Propylbenzene 104-51-8, Butylbenzene 106-42-3, p-Xylene, uses 107-06-2, 1,2-Dichloroethane, uses 107-12-0, Propionitrile 108-20-3, Diisopropyl ether 108-38-3, m-Xylene, uses 108-67-8, uses 108-87-2, Methylcyclohexane **108-88-3**, **Toluene**, uses 108-90-7, Chlorobenzene, uses 109-60-4, Propyl acetate 109-66-0, Pentane, uses 109-99-9, THF, uses 110-54-3, Hexane, uses 110-82-7, Cyclohexane, uses 111-65-9, Octane, uses 123-86-4, Butyl acetate 123-91-1, 1,4-Dioxane, uses 141-78-6, Ethyl acetate, uses 142-82-5, Heptane, uses 142-96-1, Dibutyl ether 540-84-1, Isooctane 540-88-5, Tert-Butyl acetate 554-12-1, Methyl propionate 1634-04-4, Tert-Butyl methyl ether 7732-18-5, Water, uses
(prepn. of optically active chloropropanediol derivs.)

IT 1333-74-0, **Hydrogen**, reactions **7553-56-2**, Iodine, reactions 7681-52-9, Sodium hypochlorite 7726-95-6, Bromine, reactions 7778-54-3, Hypochlorous acid, calcium salt 7782-50-5, Chlorine, reactions 27735-52-0 67560-00-3
(**prepn.** of optically active chloropropanediol derivs.)

L55 ANSWER 5 OF 23 HCA COPYRIGHT 2006 ACS on STN

139:180227 Preparation of 10-hydroxy-9-(N,N-dimethylamino)methyl-5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride. Pothukuchi, Sairam; Potlapally, Rajender Kumar; Bhatraju, Sreenivasa Rao; Kotra, Narsimha Murthy; Sirisilla, Raju; Velagala, Venkata Rama Murali Krishna Reddy; Yedugani, Lingam (Reddy's Laboratories Limited, India). PCT Int. Appl. WO 2003068778 A1 20030821, 21 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-IB547 20030218. PRIORITY: IN 2002-MA127 20020218.

GI



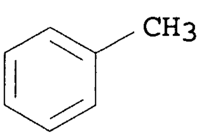
I

AB The present invention relates to a process for the prepn. of 10-hydroxy-9- (N,N-dimethylamino)methyl- 5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride (I). Thus, camptothecin reacted with K2CO2/iodine in DMF to give the 5-hydroxy deriv. which was reacted with FCH2CH2OH to give the 5-(2'-fluoroethoxy) deriv. The latter compd. was then treated with PtO2/HOAc and hydrogenated to give 10-hydroxy-5-(2'-fluoroethoxy)camptothecin (II). II reacted with HCHO/NHMe2/HOAc followed by treatment with aq. HCl to give I. Compds. like I are useful for the treatment of melanoma, prostate, leukemia, lymphoma, non-small lung cancers, cancer of the central nervous system, breast, colon, ovarian or renal cancer.

IT **108-88-3**, **Toluene**, miscellaneous
(prepn. of 10-hydroxy-9-(N,N-dimethylamino)methyl-5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride)

RN 108-88-3 HCA

CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **7553-56-2**, Iodine, reactions
(**prepn.** of 10-hydroxy-9-(N,N-dimethylamino)methyl-5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride)

RN 7553-56-2 HCA

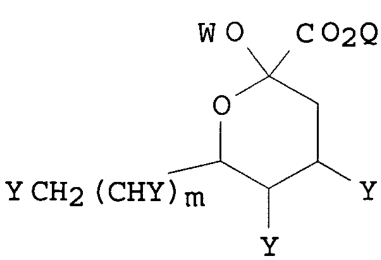
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

IC ICM C07D491-04

CC 31-5 (Alkaloids)
IT 64-17-5, Ethanol, miscellaneous 64-19-7, Acetic acid, miscellaneous 67-56-1, Methanol, miscellaneous 67-63-0, Isopropyl alcohol, miscellaneous 67-68-5, Dimethyl sulfoxide, miscellaneous 68-12-2, Dimethylformamide, miscellaneous **108-88-3**, **Toluene**, miscellaneous 617-84-5, N,N-Diethylformamide 872-50-4, 1-Methyl-2-pyrrolidinone, miscellaneous
(prepn. of 10-hydroxy-9-(N,N-dimethylamino)methyl-5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride)
IT 109-63-7, Borontrifluoride etherate 3240-34-4, Iodosobenzene diacetate 7446-70-0, Aluminum chloride, reactions 7550-45-0, Titanium tetrachloride, reactions **7553-56-2**, Iodine, reactions 7646-85-7, Zinc dichloride, reactions 7681-11-0, Potassium iodide, reactions 7722-84-1, **Hydrogen** peroxide, reactions
(**prepn.** of 10-hydroxy-9-(N,N-dimethylamino)methyl-5-(2'-fluoroethoxy)-20(S)-camptothecin hydrochloride)

L55 ANSWER 6 OF 23 HCA COPYRIGHT 2006 ACS on STN
137:370313 Process for synthesizing high-carbon monosaccharides from alkynes via halogenation and oxidation. Wu, Yulin; Li, Liansheng (Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 1309129 A **20010822**, 27 pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 2001-105412 20010223.
GI



I

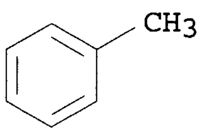
AB Title compds. I (m = 0, 1, 2; Y = OH, OAc; W = H, OAc, Me; Q = **H**, Me) are **prepd.** by halogenating ZC.tplbond.CH (Z = MeCH2(CHOR2)mCH(OR3)R4; R1 = alkyl; R2, R3 = protecting group such as ether, ester, acetal, or ketal; and R4 = alkyl) to obtain alkynyl halides, oxidizing the halides with oxidant (such as Mn(VII) compd., at a molar ratio of 1:1-5) in water-org. solvent at 0-20.degree. and pH 6-8 (adjusted with IA metal base-Mg salt) for 0.5-10 h to obtain ZCOCO2R1, removing the protecting group and cyclizing in the presence of acid (such as concd. HCl, trifluoroacetic acid, or

acetic acid), and/or acetylating with acetic anhydride or acetyl chloride in the presence of org. base (such as triethylamine, pyridine, or N,N-dimethyl-4-aminopyridine) at 20-50.degree. for 2-24 h.

IT **108-88-3**, **Toluene**, uses
(prepn. of high-carbon monosaccharides from alkynes via halogenation and oxidn.)

RN 108-88-3 HCA

CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **7553-56-2**, Iodine, reactions
(prepn. of high-carbon monosaccharides from alkynes via halogenation and oxidn.)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IC ICM C07H003-02

CC 33-2 (Carbohydrates)

IT 60-29-7, Diethyl ether, uses 71-43-2, Benzene, uses **108-88-3**, **Toluene**, uses 109-99-9, Tetrahydrofuran, uses 110-54-3, n-Hexane, uses
(prepn. of high-carbon monosaccharides from alkynes via halogenation and oxidn.)

IT 75-36-5, Acetyl chloride 98-59-9, p-Toluenesulfonyl chloride 108-24-7, Acetic anhydride 124-63-0, Methanesulfonyl chloride 128-08-5, N-Bromosuccinimide **7553-56-2**, Iodine, reactions 7722-64-7, Potassium permanganate 7726-95-6, Bromine, reactions 13824-96-9, Sodium hypobromite 13824-97-0, Potassium hypobromite 143396-26-3 148616-97-1 149128-95-0 163878-24-8 444885-23-8 448944-68-1 460325-71-7 460325-85-3 460325-86-4 460325-87-5
(prepn. of high-carbon monosaccharides from alkynes via halogenation and oxidn.)

IT 64-19-7, Acetic acid, reactions 76-05-1, Trifluoroacetic acid, reactions 109-72-8, Butyl lithium, reactions 110-18-9 110-86-1, Pyridine, reactions 110-91-8, Morpholine, reactions 110-95-2, Tetramethylpropylenediamine 121-44-8, Triethylamine, reactions 144-55-8, Sodium **hydrogen** carbonate, reactions 298-14-6 497-19-8, Sodium carbonate, reactions 554-13-2, Lithium carbonate 584-08-7, Potassium carbonate 1122-58-3,

4-Dimethylaminopyridine 4111-54-0, Lithium diisopropyl amide 5006-97-3, Lithium **hydrogen** carbonate 7087-68-5 7487-88-9, Magnesium sulfate, reactions 7558-79-4 7601-54-9, Sodium phosphate 7647-01-0, Hydrochloric acid, reactions 7758-11-4 7778-53-2, Potassium phosphate 10377-52-3, Lithium phosphate 33943-39-4, Phosphoric acid, dilithium salt
(**prepn.** of high-carbon monosaccharides from alkynes via halogenation and oxidn.)

L55 ANSWER 7 OF 23 HCA COPYRIGHT 2006 ACS on STN

136:88216 Organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels. Haenel, Matthias Walter; Narangerel, Janchig; Richter, Udo-Burckhard; Rufinska, Anna (Studiengesellschaft Kohle m.b.H., Germany). PCT Int. Appl. WO 2002002719 A1 **20020110**, 38 pp. DESIGNATED STATES: W: AU, CA, JP, US, ZA; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (German). CODEN: PIXXD2. APPLICATION: WO 2001-EP7589 20010703. PRIORITY: DE 2000-10032316 20000704.

AB Hydroliquefaction of coal is carried out at 1-100 MPa H2 and 140-500.degree. in the presence of diorganohaloboranes (R2BX), organodihaloboranes (RBX2), or dihalohydroboranes (HBX2) catalysts to hydrogenated products (R = alkyl, aryl, benzyl, and aralkyl; X = F, Cl, Br, I). The haloboranes are easily formed in-situ under the reaction conditions from a halogenation agent and: (1) organoboranes (R3B), (R2BH)2, (R2BH)2, (RBH2)2, or diborane (BH3)2, or (2) metal organoborates, of structures M+[R4B]-, M+[R3BH]- M+[R2BH2]- M+[RBH3]- or M+[BH4]- (M = Li, Na, K, Cs, Rb, 1/2Mg, 1/2Ca, 1/2Sr, 1/2 Ba, 1/2Zn). Halogenation agents include elementary halogen, X2 (X = Cl, Br, I), hydrogen halides (HX), boron trihalides (BX3), titanium tetrahalides (TiX4), tin tetrahalides (SnX4), antimony trihalides (SbX3), phosphorus pentahalide (PX5), or antimony pentahalides (SbX5). Suitable feedstocks include coal (with ranks between high-volatile bituminous and anthracite), heavy oils, petroleum distn. residues, tar sands, or oil shale, in which the raw fuels are ground or pulverized and then dispersed or suspended in liq. aliph., arom., or hydroarom. solvents (e.g., benzene, **toluene**, xylene, trimethylbenzenes, and alkyl-, dialkyl-, and trialkylbenzenes).

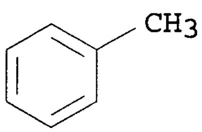
IT **7553-56-2**, Iodine, uses
(catalysts; organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **108-88-3**, **Toluene**, uses
(solvent; organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels)
RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



IC ICM C10G001-08
CC 51-21 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 29
IT Halides
Hydrogen halides
(reaction **products** with organoboranes; organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels)
IT 7429-91-6D, Dysprosium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7439-88-5D, Iridium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7439-89-6D, Iron, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7439-91-0D, Lanthanum, borohydride and organoborohydride derivs., reaction products with halogenation agents 7439-94-3D, Lutetium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7439-96-5D, Manganese, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7439-97-6D, Mercury, borohydride and organoborohydride derivs., reaction products with halogenation agents 7439-98-7D, Molybdenum, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-00-8D, Neodymium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-02-0D, Nickel, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-03-1D, Niobium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-04-2D, Osmium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-05-3D, Palladium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-06-4D, Platinum, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-10-0D, Praseodymium,

borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-12-2D, Promethium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-15-5D, Rhenium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-16-6D, Rhodium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-18-8D, Ruthenium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-19-9D, Samarium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-20-2D, Scandium, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-22-4D, Silver, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-25-7D, Tantalum, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-27-9D, Terbium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-30-4D, Thulium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-32-6D, Titanium, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-33-7D, Tungsten, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-43-9D, Cadmium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-45-1D, Cerium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-47-3D, Chromium, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-48-4D, Cobalt, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-50-8D, Copper, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-53-1D, Europium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-54-2D, Gadolinium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-57-5D, Gold, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-58-6D, Hafnium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-60-0D, Holmium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-62-2D, Vanadium, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-64-4D, Ytterbium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-65-5D, Yttrium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7440-65-5D, Yttrium, ions, borohydride and organoborohydride derivs., reaction products with halogenation agents, uses 7440-66-6D, Zinc, borohydride and organoborohydride

derivs., reaction products with halogenation agents 7440-67-7D, Zirconium, borohydride and organoborohydride derivs., reaction products with halogenation agents 7550-45-0, Titanium tetrachloride, uses **7553-56-2**, Iodine, uses 7726-95-6, Bromine, uses 7782-50-5D, Chlorine, reaction products with organoboranes or metal borohydrides 7789-68-6D, Titanium tetrabromide, reaction products with tetrapropyldiborane 13762-51-1, Potassium borohydride 16903-37-0, Borate(1-), tetrahydro-, magnesium (2:1) 16940-66-2, Sodium borohydride 16949-15-8D, Lithium borohydride, reaction products with halogenation agents 17068-95-0, Calcium borohydride 17611-70-0, Zinc borohydride 19193-36-3, Cesium borohydride 20346-99-0, Rubidium borohydride 22086-51-7D, Borane, iododipropyl-, reaction products with iodine 22784-01-6D, Tetrapropyldiborane, reaction products with iodine 42749-59-7, Strontium borohydride 52151-42-5, Barium borohydride
(catalysts; organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels)

IT 71-43-2, Benzene, uses 71-43-2D, Benzene, alkyl derivs. **108-88-3**, **Toluene**, uses 1330-20-7, Xylene, uses 25551-13-7, Trimethylbenzene
(solvent; organoborane-metal borohydride reaction products with halogenation agents as hydrogenation-hydrogenolysis catalysts for high-mol.-wt. fuels)

L55 ANSWER 8 OF 23 HCA

132:66517 Method for producing **hydrocarbons.** Kozaczko, Jozef; Syty, Zdzislaw; Gameel, Mohamed; Hanusiak, Stanislaw; Zawada, Florian (Pol.). PCT Int. Appl. WO 9967193 A1 **19991229**, 9 pp. DESIGNATED STATES: W: CA, JP, RU, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1999-PL19 19990622. PRIORITY: PL 1998-327046 19980624; PL 1999-331748 19990302.

AB This invention relates to a method for producing **hydrocarbons** with the simultaneous **prepn.** of **hydrogen** in the reaction with **iodine.** Aliph. satd. **hydrocarbons**, esp. methane or ethane, are reacted with **iodine**, this reaction being conducted preferably in the presence of a catalyst, preferably at a temp. of 400-1200.degree., with the **iodine/hydrocarbon** molar ratio of 0.1-4.0, preferably with bromine addn., preferably by activation using a method of elec. discharges and/or activation employing a method of electromagnetic radiation. After the reaction of **hydrocarbons** with **iodine**, hydrogen iodide and unreacted **iodine** are isolated from the mixt. of **hydrocarbons**, the hydrogen iodide is decompd. into **iodine** and hydrogen, the **iodine** being recycled to

the process, if needed, or hydrogen and **hydrocarbons** are sepd. and the reaction residue can be recycled to the process. In an optional soln., unsatd. **hydrocarbons** having a lower at. ratio of carbon to hydrogen are used thus obtaining **hydrocarbons** of a larger carbon/hydrogen at. ratio.

IT **74-85-1P**, Ethylene, preparation **74-86-2P**, Acetylene, preparation **1333-74-0P**, **Hydrogen**, **preparation**
(**manuf.**; method for producing **hydrocarbons** from **iodine**)

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 74-86-2 HCA
CN Ethyne (9CI) (CA INDEX NAME)

$HC{\equiv}CH$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **7553-56-2**, **Iodine**, reactions
(method for producing **hydrocarbons** from **iodine**
)

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **74-82-8**, Methane, reactions **74-84-0**, Ethane, reactions
(method for producing **hydrocarbons** from **iodine**
and)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-84-0 HCA

CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

IC ICM C07C005-44
CC 51-11 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 45, 49
ST **hydrocarbon hydrogen manuf** methane
iodination activation
IT **Hydrocarbons**, preparation
(manuf.; method for producing **hydrocarbons** from
iodine by)
IT Reactors
(membrane; in method for producing **hydrocarbons** from
iodine by iodination)
IT Iodination
(method for producing **hydrocarbons** from **iodine**
by)
IT Electric discharge
Electromagnetic wave
(method for producing **hydrocarbons** from **iodine**
under)
IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-06-4,
Platinum, uses 7440-16-6, Rhodium, uses
(catalysts contg.; method for producing **hydrocarbons**
from **iodine**)
IT **74-85-1P**, Ethylene, preparation **74-86-2P**,
Acetylene, preparation **1333-74-0P**, **Hydrogen**,
preparation
(**manuf.**; method for producing **hydrocarbons**
from **iodine**)
IT 10034-85-2, Hydrogen iodide
(method for producing **hydrocarbons** from **iodine**
)
IT **7553-56-2**, **Iodine**, reactions
(method for producing **hydrocarbons** from **iodine**
)
IT **74-82-8**, Methane, reactions **74-84-0**, Ethane,
reactions
(method for producing **hydrocarbons** from **iodine**
and)

L55 ANSWER 9 OF 23 HCA COPYRIGHT 2006 ACS on STN
130:198627 Pyrolysis of hydrocarbons in nitrogen plasma. Qiu, Jieshan;
Wang, Xiaoquan; Wang, Qian; Ma, Tengcai (Laboratory of Comprehensive
Utilization for Carbonaceous Resources Carbon Research Laboratory,
Dalian University of Technology, Dalian, Peop. Rep. China). Ranliao

Huaxue Xuebao, 26(6), 481-485 (Chinese) **1998.** CODEN:
RHXUD8. ISSN: 0253-2409. Publisher: Kexue Chubanshe.

AB The flash pyrolysis of several gaseous and liq. hydrocarbons including benzene, toluene, methane and ethane in a DC nitrogen plasma jet at atm. pressure was studied. The results show that all of the hydrocarbons used undergo fast and complex reactions with highly reactive plasma species and decomp. completely, producing a large amt. of gas and carbon black. The main components of the gas **products** are **hydrogen**, acetylene and cyanoacetylene. Some small hydrocarbons, such as methane and ethylene are also obtained in the case of benzene and toluene pyrolysis. The concn. of cyanoacetylene in the gas is related to that of acetylene. It is believed that acetylene acts as a precursor of cyanoacetylene. The carbon blacks with a narrow size distribution have a small av. diam. of 2.2-5.5 .mu.m and good adsorption capacity with an **Iodine** value of 140.apprx.180 mg.cntdot.g-1. The FTIR spectra reveal that there exist some arom. C-C bonds and a large amt. of nitrogen-contg. functional groups in the carbon blacks, such as =NH and -CN groups.

IT **1333-74-0P, Hydrogen, preparation**
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black prepn.)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **74-82-8**, Methane, reactions **74-85-1**, Ethene, reactions **74-86-2**, Acetylene, reactions
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black prepn.)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-85-1 HCA

CN Ethene (9CI) (CA INDEX NAME)

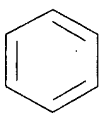
$H_2C{=}CH_2$

RN 74-86-2 HCA

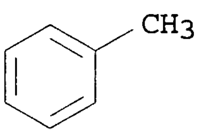
CN Ethyne (9CI) (CA INDEX NAME)

$HC \equiv CH$

IT 71-43-2, Benzene, reactions 108-88-3, Toluene,
reactions
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black
prepn.)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



CC 51-19 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 49
IT **1333-74-0P, Hydrogen, preparation**
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black
prepn.)
IT **74-82-8**, Methane, reactions **74-85-1**, Ethene,
reactions **74-86-2**, Acetylene, reactions
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black
prepn.)
IT **71-43-2**, Benzene, reactions **108-88-3**, Toluene,
reactions
(pyrolysis of hydrocarbons in nitrogen plasma and carbon black
prepn.)

L55 ANSWER 10 OF 23 HCA COPYRIGHT 2006 ACS on STN
124:353730 Kinetics of iodination of some amine-boranes with molecular
iodine in **toluene.** Das, Mrinal Kanti; Saha, Ujala;
Banerjee, Rupendranath (Dep. Chem., Jadavpur Univ., Calcutta, 700
032, India). Indian Journal of Chemistry, Section A: Inorganic,
Bio-inorganic, Physical, Theoretical & Analytical Chemistry, 35A(6),
513-516 (English) **1996.** CODEN: ICACEC. ISSN: 0376-4710.
Publisher: Publications & Information Directorate, CSIR.

AB R3N.BH3 (R = Me, Et, Prn) at room temp. reacts with I2 in **toluene** quant. to produce R3N.BHI2 when concns. of the reactants are kept low. But with reactant concns. .gtoreq. 50 mmol dm-3, R3N.NH2I and **H2** are **produced** as obsd. earlier (Inorg Synth, 12 (1970) 120). A reaction scheme has been proposed to explain this difference. Prodn. of R3N.BHI2 from R3N.BH3 proceeds in two consecutive steps: R3N.BH3 k1.fwdarw. R3N.BH2I k2.fwdarw. R3N.BHI2. Both steps are first order each in [borane] and [I2]. K1 is greater than k2 but both increase in the order Et>Me>Prn. The secondary amine-borane (Et)2NH.BH3 reacts with I2 much faster than any of the three tertiary amine-boranes studied. The obsd. order of reactivity of amine-boranes with homopolar I2 is the same as that obsd. by earlier workers with heteropolar HOCl. A bimol. mechanism with a four-membered transition state and pentacoordinate B is proposed and the sequence of reactivity appears to be primarily a result of steric influence, though electronic effects might have a modifying role.

IT **7553-56-2**, Iodine, reactions
(kinetics of iodination of amine-boranes with mol. iodine in **toluene**)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

IT Iodination
(mechanism; of amine-boranes with mol. iodine in **toluene**)

IT Kinetics of iodination
(of amine-boranes with mol. iodine in **toluene**)

IT 15112-87-5 25741-81-5 176902-47-9
(kinetics of iodination of amine-boranes with mol. iodine in **toluene**)

IT 75-22-9 1722-26-5 **7553-56-2**, Iodine, reactions 15201-50-0
(kinetics of iodination of amine-boranes with mol. iodine in **toluene**)

L55 ANSWER 11 OF 23 HCA

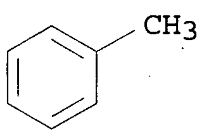
107:136342 Process for preparing para-substituted halobenzene derivatives. Sekizawa, Kazuhiko; Hironaka, Toshio; Nakano, Masao; Tsutsumi, Yukihiro (Toyo Soda Mfg. Co., Ltd., Japan). Eur. Pat. Appl. EP 231133 A1 **19870805**, 20 pp. DESIGNATED STATES: R: DE, FR, GB, NL. (English). CODEN: EPXXDW. APPLICATION: EP 1987-300884 19870202. PRIORITY: JP 1986-19693 19860131.

AB Para-substituted halobenzene derivs., useful as intermediates in the manuf. of medicines and agricultural chems. (no data), are prepd. by halogenating C6H6 or a benzene deriv. in the liq. phase in the presence of an L-type zeolite catalyst which comprises 10-95% anhyd. L-zeolite and 5-90% amorphous SiO2 as binder. A halogenation catalyst was prepd. by mixing an L-type zeolite 100, SiO2 sol (SiO2 content 30%) 15, and H2O 65 parts to form a homogeneous slurry which was spray dried, molded into a granular catalyst, and calcined in air at 600.degree. for 1 **h**, **producing** a catalyst having 87% L-type zeolite content, which when used with Cl to chlorinate PhCl produced 66.9% PhCl conversion after 3 h with 87.8% selectivity for 1,4-Cl2C6H4 and 11.2% selectivity to 1,2-Cl2C6H4, vs. 67.3, 70.3, and 27.6, resp., for a control catalyst contg. only Al2O3 as the binder.

IT **108-88-3**, **Toluene**, reactions
(halogenation of, para-selective, zeolite catalysts for)

RN 108-88-3 HCA

CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **7553-56-2**, Iodine, reactions
(iodination by, para-selective, of benzene (derivs.), zeolite catalysts for)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IC ICM C07C025-02
ICS C07C017-12; B01J029-28

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 5, 25, 63, 67

IT **108-88-3**, **Toluene**, reactions
(halogenation of, para-selective, zeolite catalysts for)

IT **7553-56-2**, Iodine, reactions
(iodination by, para-selective, of benzene (derivs.), zeolite catalysts for)

L55 ANSWER 12 OF 23 HCA COPYRIGHT 2006 ACS on STN

96:143009 Mechanistic study of photoinduced .beta.-hydride elimination. The facile photochemical synthesis of low-valent thorium and uranium organometallics. Bruno, Joseph W.; Kalina, Dale G.; Mintz, Eric A.;

Marks, Tobin J. (Dep. Chem., Northwestern Univ., Evanston, IL, 60201, USA). Journal of the American Chemical Society, 104(7), 1860-9 (English) **1982.** CODEN: JACSAT. ISSN: 0002-7863.

AB A mechanistic investigation of the photochem. of RTh(C5E5)3 (I; R = Me, Me2CH, Bu; C5E5 = cyclopentadienyl; E = H, D), Me2CHTh(MeC5H4)3, BuTh(indenyl)3, RU(C5E5)3 (E = H, R = Me, Me2CH, Bu, EtCHMe; E = D, R = Br) was reported. For I (R = Me), UV photolysis in arom. solvents produces 1:1 alkane-alkene (RH:R - H) mixts. with the trivalent complex Th(C5E5)3 in nearly stoichiometric yield. On the basis of products, product yields, labeling studies, matrix photochem., added reagents, and the behavior of these compds., a photoinduced .beta.-H elimination mechanism is proposed. This reaction yields (irreversibly) olefin and HTh(C5E5)3, the latter species then reacting with another I mol. to produce alkane and Th(C5E5)3. A minor pathway for RH formation involves abstraction of C5E5 or solvent H (D) atoms. On the basis of spectroscopic, magnetic, and chem. studies, the Th photoproduct is formulated as a Th(.eta.5-C5E5)3 compd., possibly with metal-bridging cyclopentadienyl ligands in the solid state. In contrast to these results, photolysis of the indenyl compd. produces only alkane, the added H atom being derived from the indenyl ligand. For the U compds. in arom. solvents, photoinduced .beta.-H elimination [and U(C5H5)3 formation)] occurs but is not the major pathway. Rather, H-atom abstraction from cyclopentadienyl rings (analogous to the thermolysis pathway) predominates, with lesser abstraction from the solvent mols. Photolysis in THF greatly increases the yield of U(C5H5)3.

IT **74-82-8P**, preparation **74-84-0P**, preparation
74-98-6P, preparation **106-97-8P**, preparation
106-98-9P, preparation **115-07-1P**, preparation
590-18-1P 624-64-6P 1333-74-0P,
preparation
(prepn. of, by photolysis of organoactinide)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

$H_3C—CH_3$

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 106-98-9 HCA
CN 1-Butene (8CI, 9CI) (CA INDEX NAME)

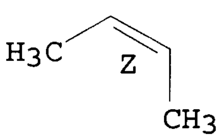
$H_3C-CH_2-CH=CH_2$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

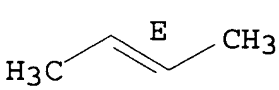
RN 590-18-1 HCA
CN 2-Butene, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 624-64-6 HCA
CN 2-Butene, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

$H-H$

IT **7553-56-2**, reactions

(reaction of, with tris(cyclopentadienyl)thorium)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **501-65-5**
(reaction of, with tris(cyclopentadienyl)thorium Me complex)
RN 501-65-5 HCA
CN Benzene, 1,1'-(1,2-ethynediyl)bis- (9CI) (CA INDEX NAME)

Ph—C≡C—Ph

CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22
IT **74-82-8P**, preparation **74-84-0P**, preparation
74-98-6P, preparation **106-97-8P**, preparation
106-98-9P, preparation **115-07-1P**, preparation
590-18-1P **624-64-6P** **1333-74-0P**,
preparation
(prepn. of, by photolysis of organoactinide)
IT 80410-12-4P
(prepn. of, by reaction of cyclopentadienylthorium with
iodine)
IT 66775-24-4P
(prepn. of, by reaction of tris(indenyl)thorium with
iodine)
IT 67-56-1, reactions 67-66-3, reactions **7553-56-2**,
reactions 12125-02-9, reactions
(reaction of, with tris(cyclopentadienyl)thorium)
IT **501-65-5**
(reaction of, with tris(cyclopentadienyl)thorium Me complex)

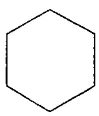
L55 ANSWER 13 OF 23 HCA COPYRIGHT 2006 ACS on STN
91:41471 **Manufacture** of **hydrogen** by thermal
decomposition of hydrogen sulfide. Kameyama, Tetsuya; Dokiya,
Masayuki; Fukuda, Kenzo (Agency of Industrial Sciences and
Technology, Japan). Jpn. Kokai Tokkyo Koho JP 54016395
19790206 Showa, 3 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 1977-81154 19770707.
AB H2S is reacted with 12 in the presence of H2O to give HI, which is
then reacted with arom. compds. in the presence of Ru to give
hydrogenated arom. compds., and dehydrogenation of the hydrogenated
compds. gives H2 and recovers the arom. compds. Thus, H2S was
reacted with **I2** in the presence of H2O at 50.degree. to
give HI, which was then reacted with **C6H6** in the presence

of Ru hydroxide at 150.degree. to give **cyclohexane.**
Catalytic dehydrogenation of the **cyclohexane** at
300.degree. with Pt supported by Al2O3 gave H2.

IT **110-82-7P**, preparation
(formation and dehydrogenation of, in **hydrogen manuf.** from **hydrogen** sulfide)

RN 110-82-7 HCA

CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT **1333-74-0P**, preparation
(**manuf.** of, from **hydrogen** sulfide)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **7553-56-2**, reactions
(reaction of, with hydrogen sulfide, in **hydrogen manuf**)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IC C01B001-03; C01B017-06

CC 49-1 (Industrial Inorganic Chemicals)

ST **hydrogen manuf**; sulfide hydrogen decompn
iodine; **cyclohexane** dehydrogenation

IT **110-82-7P**, preparation
(formation and dehydrogenation of, in **hydrogen manuf.** from **hydrogen** sulfide)

IT 10034-85-2P
(formation and reaction of, in **hydrogen manuf**. from **hydrogen** sulfide)

IT **1333-74-0P**, preparation
(**manuf.** of, from **hydrogen** sulfide)

IT **7553-56-2**, reactions
(reaction of, with hydrogen sulfide, in **hydrogen manuf**)

IT 7783-06-4, reactions

(reaction of, with **iodine** in **hydrogen manuf**)

L55 ANSWER 14 OF 23 HCA COPYRIGHT 2006 ACS on STN
84:82455 Radiation formation of methyl iodide. II. Chain decomposition of methane-**iodine** mixtures at elevated temperatures.
Bartonicek, B.; Hladky, E.; Schweiner, Z.; Bednar, J. (Nucl. Res. Inst., Rez., Czech.). Mech. Hydrocarbon React., Symp., Meeting Date 1973, 695-702. Editor(s): Marta, F.; Kallo, D. Elsevier: Amsterdam, Neth. (English) **1975.** CODEN: 31VWAH.

AB Gaseous CH4-I mixts. decomp. under the action of .gamma.-radiation and (or) by heating. The main decompn. products are MeI, HI, C2H4, and mol. H, the latter being formed only by irradn. While the radiation decompn. is a nonchain process at the room temp., an increase of temp. brings about a radiolytic and thermal chain formation of MeI and HI. MeI contributes, by its thermal decompn., to the initiation and propagation of this chain reaction. Below .apprx.450.degree., H atoms do not have any effect on the thermal chain decompn. of these mixts. Since even MeI decomps. by heat, the only I-contg. product above .apprx.400.degree. is HI.

IT **74-85-1P**, preparation **1333-74-0P**, preparation
(formation of, from radiolysis of **iodine**-methane gaseous mixts. at elevated temps.)

RN 74-85-1 HCA

CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **74-82-8**, reactions
(radiolysis of gaseous mixts. of **iodine** and, at elevated temps., chain reaction mechanism of)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

IT **7553-56-2**, reactions
(radiolysis of gaseous mixts. of methane and, at elevated temps., chain reaction mechanism of)

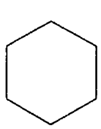
RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic
 Processes)
ST radiolysis methane **iodine** mixt
IT Radiolysis
 (of **iodine**-methane gaseous mixts. at elevated temps.,
 chain reaction mechanism fof)
IT **74-85-1P**, preparation 74-88-4P **1333-74-0P**,
 preparation 10034-85-2P
 (formation of, from radiolysis of **iodine**-methane
 gaseous mixts. at elevated temps.)
IT **74-82-8**, reactions
 (radiolysis of gaseous mixts. of **iodine** and, at
 elevated temps., chain reaction mechanism of)
IT **7553-56-2**, reactions
 (radiolysis of gaseous mixts. of methane and, at elevated temps.,
 chain reaction mechanism of)

L55 ANSWER 15 OF 23 HCA COPYRIGHT 2006 ACS on STN
84:37265 Radiolysis of **cyclohexane**-hexamethylbenzene mixtures.
 II. Experiments with scavengers. Roder, Magdolna (Cent. Res. Inst.
 Phys., Budapest, Hung.). Acta Chimica Academiae Scientiarum
 Hungaricae, 86(3), 211-18 (English) **1975**. CODEN: ACASA2.
 ISSN: 0001-5407.
AB The 60Co .gamma.-radiolysis of **cyclohexane**
 (I)-hexamethylbenzene (II) mixts. was investigated in the presence
 of the scavengers I, N2O, CCl4, and cyclo-C3H6. The radiation chem.
 yields of H, N, and C3H8 were detd. as a function of compn. The
 protective effect of II on the I radiolytic decompn. is accounted
 for mainly (.apprx.90%) by the transfer of pos. charge from I mol.
 cations to II. The remaining 10% is probably caused by excitation
 energy transfer.
IT **34473-67-1P**, preparation
 (formation of, in radiolysis of **cyclohexane**
 -hexamethylbenzene mixts., energy transfer in)
RN 34473-67-1 HCA
CN Cyclohexane, radical ion(1+) (9CI) (CA INDEX NAME)



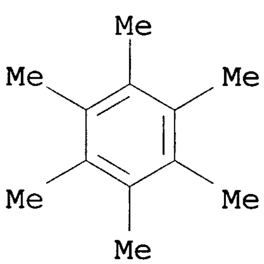
IT **74-98-6P**, preparation **1333-74-0P**, preparation
(formation of, in radiolysis of **cyclohexane**
-hexamethylbenzene mixts., scavenger effect on)
RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

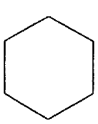
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **87-85-4**
(radiolysis of mixts. of **cyclohexane** and, scavenger
effect on)
RN 87-85-4 HCA
CN Benzene, hexamethyl- (8CI, 9CI) (CA INDEX NAME)



IT **110-82-7**, reactions
(radiolysis of mixts. of hexamethylbenzene and, scavenger effect
on)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT **75-19-4 7553-56-2**, uses and miscellaneous
(scavenger, in radiolysis of **cyclohexane**
-hexamethylbenzene mixts.)
RN 75-19-4 HCA
CN Cyclopropane (8CI, 9CI) (CA INDEX NAME)

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
ST radiolysis **cyclohexane** hexamethylbenzene
IT Energy level excitation
(in **cyclohexane**, radiolysis in relation to)
IT Energy transfer
(in radiolysis of **cyclohexane**-hexamethylbenzene mixts.)
IT Radiolysis
(of **cyclohexane**-hexamethylbenzene mixts., scavenger effect on)
IT **34473-67-1P**, preparation
(formation of, in radiolysis of **cyclohexane** -hexamethylbenzene mixts., energy transfer in)
IT **74-98-6P**, preparation **1333-74-0P**, preparation 7727-37-9P, preparation
(formation of, in radiolysis of **cyclohexane** -hexamethylbenzene mixts., scavenger effect on)
IT **87-85-4**
(radiolysis of mixts. of **cyclohexane** and, scavenger effect on)
IT **110-82-7**, reactions
(radiolysis of mixts. of hexamethylbenzene and, scavenger effect on)
IT 56-23-5, uses and miscellaneous **75-19-4** **7553-56-2** , uses and miscellaneous 10024-97-2, uses and miscellaneous
(scavenger, in radiolysis of **cyclohexane** -hexamethylbenzene mixts.)

L55 ANSWER 16 OF 23 HCA
83:50649 Radiolysis of **cyclohexane**-hexamethyl-benzene mixtures. **I. Pure** substances. Roder, Magda (Cent. Res. Inst. Phys., Budapest, Hung.). Acta Chimica Academiae Scientiarum Hungaricae, 85(1), 55-62 (English) **1975.** CODEN: ACASA2. ISSN: 0001-5407.
AB The 60Co .gamma.-radiolysis of **cyclohexane** -hexamethylbenzene mixts. with 0-100% hexamethylbenzene was investigated in the liq. and solid phases. The radiation chem.

yields of H2 and CH4 were detd. as a function of the mixt. compn. and temp., -196 to +170.degree.. Hexamethylcyclohexane has a protective effect on **cyclohexane** decompn. in the liq. phase; this effect can be understood in terms of some kind of phys. interaction.

IT **1333-74-0P**, preparation
(formation of, in radiolysis of **cyclohexane** -hexametehylbenzene mixts., hexamethylbenzene protective effect in relation to)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **74-82-8**, preparation
(formation of, in radiolysis of **cyclohexane** -hexametehylbenzene mixts., hexamethylbenzene protective effect in relation to)

RN 74-82-8 HCA

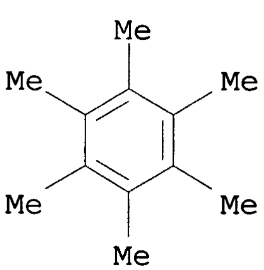
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

IT **87-85-4**
(radiolysis of **cyclohexane** and, hexamethylbenzene protective effect in)

RN 87-85-4 HCA

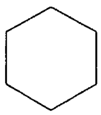
CN Benzene, hexamethyl- (8CI, 9CI) (CA INDEX NAME)



IT **110-82-7**, reactions
(radiolysis of hexamethylbenzene and, hexamethylbenzene protective effect in)

RN 110-82-7 HCA

CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
ST **cyclohexane** methylbenzene radiolysis; irradn gamma **cyclohexane** methylbenzene
IT Radiolysis
(of **cyclohexane**-hexamethylbenzene mixts., hexamethylbenzene protective effect in)
IT **1333-74-0P**, preparation
(formation of, in radiolysis of **cyclohexane** -hexametehylbenzene mixts., hexamethylbenzene protective effect in relation to)
IT **74-82-8**, preparation
(formation of, in radiolysis of **cyclohexane** -hexametehylbenzene mixts., hexamethylbenzene protective effect in relation to)
IT **87-85-4**
(radiolysis of **cyclohexane** and, hexamethylbenzene protective effect in)
IT **110-82-7**, reactions
(radiolysis of hexamethylbenzene and, hexamethylbenzene protective effect in)

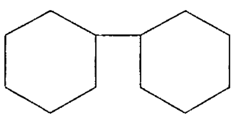
L55 ANSWER 17 OF 23 HCA COPYRIGHT 2006 ACS on STN
80:102245 Effect of **iodine** as a radical scavenger in the .gamma. radiolysis of liquid-phase **cyclohexane** -perfluorocyclohexane solutions. Kennedy, George A.; Hanrahan, Robert J. (Dep. Chem., Univ. Florida, Gainesville, FL, USA). Journal of Physical Chemistry, 78(4), 366-71 (English) **1974** . CODEN: JPCHAX. ISSN: 0022-3654.
AB The effects of **I2** as a radical scavenger in the .gamma.-radiolysis of liq. cyclo-**C6H12**-cyclo-C6F12 mixt. at 65.degree. were studied. Both **I2** consumption (with added **I2**) and **I2** prodn. (with added HI) gave reliable radical counting over most of the concn. range. The total radical yields were .apprx.6.0 for both of the pure compds. and a max. of .apprx.9.0 for solns. contg. 30 electron % cyclo-C6F12. With resp. to the hydrocarbon products, both the qual. and quant. effects of added **I2** agree with simple expectations; the disproportionation/combination products (cyclohexene and dicyclohexyl) from cyclohexyl radicals are sharply reduced, and a substantial yield of cyclo-C6H11I is formed, showing a max. yield of

7.2 which is nearly const. from 10 to 60 electron % cyclo-C6F12. The H2 yield, which is strongly depressed by the fluorocarbon, shows little further effect of the added **I2.** The yield of cyclo-C6-HF11 is essentially unaffected by added **I2**, in spite of the fact that **I2** is a good scavenger of cyclo-C6F11 radicals in pure cyclo-C6F12. The (thermal) cyclo-C6F11 radical is not a precursor of cyclo-C6HF11 in the irradiated mixts. Addnl. photolytic expts. on solns. contg. HI (as a source of H atoms) and Ph3N (as a source of photoelectrons) suggest, resp., that H atoms are not involved, and that electrons or neg. ions are involved, in C-F bond rupture.

IT **92-51-3P 110-83-8P**, preparation **1333-74-0P**
, preparation
(formation of, in radiolysis of **cyclohexane**
-perfluorocyclohexane mixts. in presence of **iodine**)

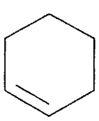
RN 92-51-3 HCA

CN 1,1'-Bicyclohexyl (9CI) (CA INDEX NAME)



RN 110-83-8 HCA

CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

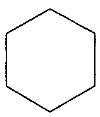
IT **7553-56-2**, uses and miscellaneous
(radiolysis of **cyclohexane**-perfluorocyclohexane liq. mixt. in presence of, radical scavenging in)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **110-82-7**, reactions
(radiolysis of perfluorocyclohexane and, **iodine** effect on radical formation in)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
ST **cyclohexane** radiolysis **iodine** effect; perfluorocyclohexane radiolysis **iodine** effect; radical scavenging **cyclohexane** radiolysis
IT Radiolysis
(of **cyclohexane**-perfluorocyclohexane liq. **mixt**., **iodine** radical scavenger effect in)
IT 7664-39-3P, preparation
(formation of, in radiolysis of **cyclohexane**-perfluorocyclohexane mixts.)
IT **92-51-3P** **110-83-8P**, preparation 308-24-7P 626-62-0P **1333-74-0P**, preparation
(formation of, in radiolysis of **cyclohexane**-perfluorocyclohexane mixts. in presence of **iodine**)
IT 355-68-0
(radiolysis of **cyclohexane** and, **iodine** effect on radical formation in)
IT 603-34-9 **7553-56-2**, uses and miscellaneous 10034-85-2
(radiolysis of **cyclohexane**-perfluorocyclohexane liq. mixt. in presence of, radical scavenging in)
IT **110-82-7**, reactions
(radiolysis of perfluorocyclohexane and, **iodine** effect on radical formation in)

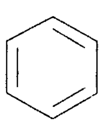
L55 ANSWER 18 OF 23 HCA COPYRIGHT 2006 ACS on STN
71:34972 Radiolysis of alcohols at low temperatures. I. The precursors of hydrogen in glassy methanol. Teply Jiri; Janovsky, Igor (Inst. Nucl. Res., Rez/Prague, Czech.). International Journal for Radiation Physics and Chemistry, 1(2), 119-31 (English) **1969**. CODEN: IJRCA6. ISSN: 0020-7055.
AB By using various electron and H atom scavengers the .gamma.-irradn. yields of different H precursors in glassy photobleached MeOH were detd.: the yields of the trapped electrons, of the independently **formed H** atoms, of the hot H atoms, and of the "molecularly" **formed H** are 2.3, .apprx. 0.5,

.apprx.1.1, and .apprx.0.3, resp. Some conclusions about the sepn. of electrons from their conjugated ions are drawn from the comparison of these yields with those for liq. MeOH. In acid MeOH glass G(H2) is larger by 0.5 than in neutral glass. A possible explanation is offered, namely, that a low excited state of MeOH is decompd. by the influence of the elec. field of the ions. When the irradiated MeOH glass is warmed in the dark, thermally bleached, the yields of H and glycol are smaller but the reasons for this are not quite clear. Also the cryst. MeOH gives questionable results. A few remarks on the process of electron trapping are added.

IT **1333-74-0P**, preparation
(formation of, in methanol glasses radiolysis)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **71-43-2**, reactions **111-66-0 115-07-1**, reactions **7553-56-2**, reactions
(radiolysis of methanol glasses and)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 111-66-0 HCA
CN 1-Octene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH-(CH_2)_5-Me$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH{=}CH_2$

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

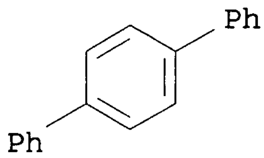
I—I

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT Radiolysis
(of methanol glasses, **hydrogen formation** in)
IT **1333-74-0P**, preparation 12385-13-6P, preparation
(formation of, in methanol glasses radiolysis)
IT 67-56-1, reactions
(radiolysis of glasses of, **hydrogen formation**
in)
IT 56-23-5, reactions **71-43-2**, reactions 107-18-6,
reactions **111-66-0** **115-07-1**, reactions
7553-56-2, reactions 7647-01-0, reactions 7664-93-9,
reactions
(radiolysis of methanol glasses and)

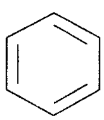
L55 ANSWER 19 OF 23 HCA COPYRIGHT 2006 ACS on STN
71:8392 Effect of luminescent additives on the radiation yield of
hydrogen during the radiolysis of aromatic solvents. Gurskii, M.
N.; Tsoi, A. N. (Inst. Yad. Fiz., Tashkent, USSR). Khimiya Vysokikh
Energii, 3(2), 187-8 (Russian) **1969.** CODEN: KHVKAO.
ISSN: 0023-1193.
AB The radiation yield of H in the radiolysis of benzene (I) and
toluene (II) in the presence of n-terphenyl (III) was studied at
60Co .gamma.-ray doses of 6 .times. 1017-1020 ev./cm.3 The concn. of
the products of radiolysis does not exceed that of the luminescent
additive (Cprod .ltoreq. 10-2M). Accumulation of H as a function of
dose is linear for irradn. of **pure I.** Addn. of
III decreases the amt. of **H formed.** An
analogous effect is observed with II. The shielding effect, as
detd. from the H yield, is observed only at low irradn. doses.
Increase in the integral dose increases the H yield. At a dose
where the concn. of the products of radiolysis is comparable to that
of the luminescent additive no shielding effect is observed. If the
III concn. is increased to 2 .times. 10-2 M the H yield decreases
with an efficiency of 400 1./mole.
IT **1333-74-0P**, preparation
(formation of, in radiolysis of aromatic hydrocarbons)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

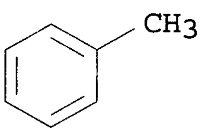
IT **92-94-4**
(radiolysis of aromatic hydrocarbons and, **hydrogen**
formation in)
RN 92-94-4 HCA
CN 1,1':4',1''-Terphenyl (9CI) (CA INDEX NAME)



IT 71-43-2, reactions 108-88-3, reactions
(radiolysis of terphenyl and, **hydrogen formation** in)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT Radiolysis
(of aromatic hydrocarbon-terphenyl mixts., **hydrogen formation** in)
IT **1333-74-0P**, preparation
(formation of, in radiolysis of aromatic hydrocarbons)
IT **92-94-4**
(radiolysis of aromatic hydrocarbons and, **hydrogen formation** in)
IT **71-43-2**, reactions **108-88-3**, reactions
(radiolysis of terphenyl and, **hydrogen formation** in)

L55 ANSWER 20 OF 23 HCA COPYRIGHT 2006 ACS on STN
70:33202 Steric effect in the radiolysis of cis- and trans-1,2-dimethylcyclohexane. Eberhardt, Manfred K. (Puerto Rico Nucl. Center, Rio Piedras, P. R.). Journal of Physical Chemistry, 72(13), 4509-12 (English) **1968**. CODEN: JPCHAX. ISSN: 0022-3654.
AB The radiolysis of cis- and trans-1,2-dimethylcyclohexane in the liq.

phase was studied from 2 .times. 1020 to 16 .times. 1020ev./ml. at a dose rate of 8.3 .times. 1018 ev./ml.hr. The main **products** are **H2**, 1,2-dimethylcyclohexene, 2,3-dimethylcyclohexene, 3,4-dimethylcyclohexene, 4,5-dimethylcyclohexene, 2-octene, dimeric products, and isomerization. The trans compd. shows a greater decrease in G(olefin) with increasing dose than the cis isomer. **Iodine** (2 .times. 10-2 M) reduces G(H2) in the trans-1,2-dimethylcyclohexane from 3.54 to 2.36 (.DELTA.(G(H2)) = 1.18) but in the cis isomer the G(H2) is only reduced from 3.70 to 3.05 (.DELTA.(G(H2)) = 0.65). These results suggest that the difference of unscavengeable H between the two isomers, 3.05 - 2.36 = 0.69, is due to mol. H elimination in the cis-1,2-dimethylcyclohexane and that tertiary axial hydrogens lead preferentially to the **formation** of scavengeable **hydrogen** atoms. A similar behavior was observed with cis- and trans-Decalin. Evidence for opening and reclosure of the **cyclohexane** ring is presented.

IT **111-67-1P 1333-74-0P**, preparation
1674-10-8P 1759-64-4P 2808-72-2P
3685-00-5P
(formation of, in radiolysis of dimethylcyclohexane)

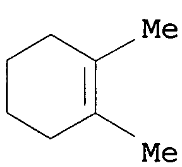
RN 111-67-1 HCA
CN 2-Octene (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-CH=CH-Me$

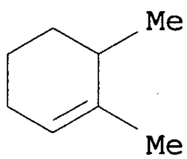
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

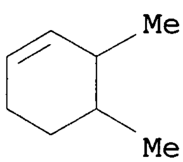
RN 1674-10-8 HCA
CN Cyclohexene, 1,2-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 1759-64-4 HCA
CN Cyclohexene, 1,6-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

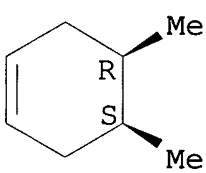


RN 2808-72-2 HCA
CN Cyclohexene, 3,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 3685-00-5 HCA
CN Cyclohexene, 4,5-dimethyl-, cis- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.

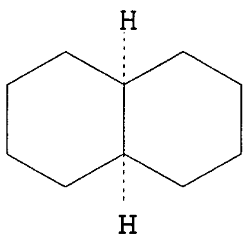


IT **7553-56-2**, uses and miscellaneous
(radiolysis of dimethylcyclohexane in presence of, **hydrogen formation** in relation to)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

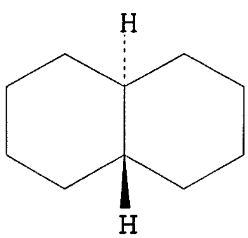
IT **493-01-6 493-02-7 2207-01-4**
6876-23-9
(radiolysis of, steric effects in)
RN 493-01-6 HCA
CN Naphthalene, decahydro-, cis- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.



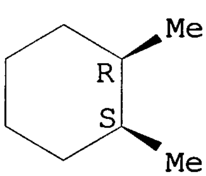
RN 493-02-7 HCA
CN Naphthalene, decahydro-, trans- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.



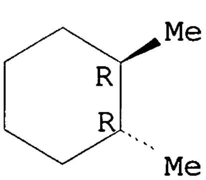
RN 2207-01-4 HCA
CN Cyclohexane, 1,2-dimethyl-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 6876-23-9 HCA
CN Cyclohexane, 1,2-dimethyl-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
ST steric effect; **cyclohexanes** radiolysis; radiolysis **cyclohexanes**; methylcyclohexanes radiolysis; dimethylcyclohexane radiolysis
IT **111-67-1P 1333-74-0P**, preparation
1674-10-8P 1759-64-4P 2808-72-2P
3685-00-5P
(formation of, in radiolysis of dimethylcyclohexane)
IT **7553-56-2**, uses and miscellaneous
(radiolysis of dimethylcyclohexane in presence of, **hydrogen formation** in relation to)
IT **493-01-6 493-02-7 2207-01-4**
6876-23-9
(radiolysis of, steric effects in)

L55 ANSWER 21 OF 23 HCA
70:24672 Behavior of tritium recoil atoms in solid **mixtures** of **cyclohexane** and **benzene** with **iodine** additives. Avdonina, E. N.; Nesmeyanov, A. N. (USSR). Radiokhimiya, 10(5), 568-74 (Russian) **1968**. CODEN: RADKAU. ISSN: 0033-8311.
AB The effect of addns. and changes in the aggregate state on stabilization of T recoil atoms in binary mixts. of cyclohexane with benzene was studied. Irradn. of the mixts. with addn. of 3.2 .times. 10-4, 3.8 .times. 10-3, 5 .times. 10-2 M iodine was carried out in quartz ampuls for 2 hrs. at 9 .times. 1011 n/cm.2-sec. The principal stable formations are HT, the labeled mother compds., and high-boiling products. The probability of HT formation in benzene is 6.4%. In the interaction with solid benzene, 73% of T recoil atoms is stabilized. In pure cyclohexane the HT yield is 60%. In a cyclohexane mol. .apprx.22% of recoil atoms is stabilized. The probability of splitting-off of **H** with **formation** of HT in the solid phase is lower: the yield of HT from benzene by a factor of 2.5, and from cyclohexane by a factor of 0.1 compared with the liq. phase. The presence of iodine in amts. of (3-4) .times. 10-4 M has practically no effect on the yield of labeled products in all solid systems studied. With 5 .times. 10-2 M the HT yield increases noticeably with benzene concns. from 10 to 40 mole %. For cyclohexane-rich mixts. and for pure benzene the HT yield is the same as without I. The most important component of the high-boiling fractions are heavy polymers, nonvolatile at room temp. and 10-2 torr. In-crease in the concn. of the aromatic component, transition from the liq. to the solid state, and the presence of iodine increases the probability of stabilization in mother mols. and in satd. and aromatic hydrocarbons.
CC 75 (Nuclear Phenomena)

L55 ANSWER 22 OF 23 HCA

63:7033 Original Reference No. 63:1258b-c Investigations on parachor. Vaidya, V. G. (Holkar Coll., Indore, India). Agra University Journal of Research, Science, 12(1), 313-16 From: CZ 1964(39), Abstr. No.578. (English) **1963.** CODEN: AURSA9. ISSN: 0002-1032.

AB The applicability of the mixt. rule of Hammick and Andrew was checked. The complex formation was investigated in the systems Pb(NO3)2-glycine, Co(NO3)2-glycine, CrO42--Cr2O72-, C6H6-I, and alc.-I and the H bond of HNO3, H2SO4, H3PO4, and H3BO3 through detn. of the parachors of these compds. in the pure and dild.states.

CC 6 (Phase Equilibriums, Chemical Equilbriums, and Solutions)

IT Parachors
(in complex **formation** and **H** bond studies)

IT 7553-56-2, **Iodine**
(**mixts.** with **benzene** and EtOH, parachor in relation to)

L55 ANSWER 23 OF 23 HCA COPYRIGHT 2006 ACS on STN

56:11361 Original Reference No. 56:2099i,2100a Radiation chemistry of cyclohexane, III. Effect of **benzene** and **iodine** on the isotopic **composition** of radiolytic H from C6D12-C6H12 mixtures. Dyne, P. J.; Jenkinson, W. M. (At. Energy Canada, Ltd., Chalk River). Canadian Journal of Chemistry, 39, 2163-70 (Unavailable) **1961.** CODEN: CJCHAG. ISSN: 0008-4042.

AB cf. CA 54, 20444b. The isotopic compn. of H evolved in the radiolysis of C6D12-C6H12 mixts. is changed by the addn. of benzene and I. The unimol. yield of D is 0.32 .+-. 0.02 moles/100 e.v. This is reduced by additives. The value of f = (HD)2/(H2)(D2) increases linearly with C6D12 concn., and is approx. 1.0 at 10 mole % C6D12. Benzene increases f while I decreases f slightly. Thus I and benzene suppress both unimol. and bimol. decompn. modes to a comparable extent, suggesting that both act by quenching a common precursor.

CC 11 (Radiation Chemistry and Photochemistry)

IT Radiation and Radiation effects
(decompn. by, of cyclohexane mixt. with C6D12, effect of benzene and I on isotopic compn. of **H formed** therein)

IT Cyclohexane-d12, mixt. with cyclohexane
(effect of benzene and I on **H** isotopic compn. **formed** in radiolysis of)

IT 71-43-2, Benzene
(effect on **H** isotopic compn. **formed** in radiation decompn. of C6D12-C6H12 mixts.)

IT 7782-39-0, Deuterium
(**formation** of **H** and, in radiolysis of C6D12-C6H12 mixts., effect of benzene and I on)

IT 1333-74-0, **Hydrogen**

(**formation** or evolution of, from cyclohexane-d and cyclohexene by radiation, effect of benzene and I on)

IT 7553-56-2, Iodine
(hydrocarbon dehydrogenation by, **hydrogen** isotopic compn. **formed** in radiation decompn. of C6D12-C6H12 mixts. in relation to)

IT 110-82-7, Cyclohexane
(mixts. of, with cyclohexane-d12, decompn. by radiation, effect of benzene and I on isotopic compn. of **H formed** in)

=> d l56 1-16 cbib abs hitstr hitind

L56 ANSWER 1 OF 16 HCA COPYRIGHT 2006 ACS on STN

138:13889 Heavy Ion Radiolysis of Liquid Benzene. LaVerne, Jay A.; Araos, M. S. (Radiation Laboratory, University of Notre Dame, Notre Dame, IN, 46556, USA). Journal of Physical Chemistry A, 106(46), 11408-11413 (English) **2002.** CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB The mechanisms responsible for the main products in liq. benzene radiolysis (biphenyl, mol. hydrogen, and Ph radical) are probed with protons, helium ions, and carbon ions of a few to 30 MeV energy. Ph radical yields have been examd. using **iodine** scavenging techniques. The results are combined with similar data for .gamma.-rays and suggest that Ph radicals mainly react with benzene to give a long-lived adduct, which leads to polymer formation. **Iodine** can react with this adduct to give enhanced yields of biphenyl. Biphenyl is the predominant single hydrocarbon product in the radiolysis of neat benzene with a yield of 0.075 mol./100 eV. Its yield is nearly independent of radiation type and energy suggesting that its formation in neat benzene is due to a fast ion-mol. process and not due to Ph radicals. The total yield of 0.7 radicals/100 eV is almost entirely due to Ph radicals and H atoms. A reexamn. of the fluorescence from the singlet excited state of benzene suggests that this state is the precursor for mol. hydrogen and acetylene, whereas the triplet excited state decays to Ph radicals and H atoms. Most of the excited states formed in the .gamma.-radiolysis of benzene seem to decay to ground without formation of any product.

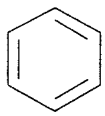
IT **7553-56-2, Iodine**, reactions
(Ph radical scavenger; heavy ion radiolysis of liq. benzene)

RN 7553-56-2 HCA

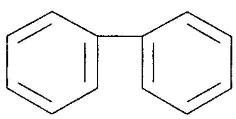
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

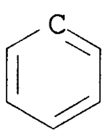
IT 71-43-2, Benzene, reactions
(heavy ion radiolysis of liq. benzene)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



IT 92-52-4, Biphenyl, formation (nonpreparative)
(heavy ion radiolysis of liq. benzene)
RN 92-52-4 HCA
CN 1,1'-Biphenyl (9CI) (CA INDEX NAME)



IT 2396-01-2, Phenyl radical
(scavenging; heavy ion radiolysis of liq. benzene)
RN 2396-01-2 HCA
CN Phenyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): 74
IT Excited singlet state
(responsible for **H2 prodn.**; heavy ion
radiolysis of liq. benzene)
IT **7553-56-2**, **Iodine**, reactions
(Ph radical scavenger; heavy ion radiolysis of liq. benzene)
IT **71-43-2**, Benzene, reactions
(heavy ion radiolysis of liq. benzene)
IT **92-52-4**, Biphenyl, formation (nonpreparative) 591-50-4,
Iodobenzene
(heavy ion radiolysis of liq. benzene)
IT **2396-01-2**, Phenyl radical
(scavenging; heavy ion radiolysis of liq. benzene)

L56 ANSWER 2 OF 16 HCA COPYRIGHT 2006 ACS on STN
130:337784 The surface chemistry of 1-iodopropane adsorbed on Pt(111).
Scoggins, Troy B.; Ihm, Hyeran; White, John M. (Center for Materials Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712, USA). Israel Journal of Chemistry, 38(4), 353-363 (English) **1998.** CODEN: ISJCAT. ISSN: 0021-2148. Publisher: Laser Pages Publishing.

AB POn Pt(111) at 110 K, 1-iodopropane, C3H7I, adsorbs molecularly, but for doses below 1.7 .times. 1014 mols. cm-2, only H2 and I appear in thermal desorption. C-I bond cleavage occurs between 160 and 220 K, forming adsorbed Pr, C(a)H2CH2CH3, and at. **iodine**, based on temp.-programmed desorption (TPD), high-resoln. electron energy loss spectroscopy (HREELS), and XPS (XPS). N-Pr undergoes .beta.-hydride elimination forming propylene, with desorption peaks at 185 and 240 K. At 240 K, hydrogenation to propane also occurs. Some di-.sigma. bonded propylene, C(a)H2C(a)HCH3, remains at 240 K and it rearranges to propylidyne near 300 K. At. H, bound to Pt, recombines and desorbs at ca. 260 K. Further desorption of H2 is limited by C-H bond breaking and occurs over a broad temp. range with local maxima at ca. 280, 320, and 420 K, typical of propylidyne fragments on Pt. At. **iodine** desorbs in a broad feature at 825 K.

IT **115-07-1D**, Propylene, adsorbed intermediate
2143-61-5D, Propyl, adsorbed intermediate
85056-54-8D, Propylidyne, adsorbed intermediate
(surface chem. of 1-iodopropane adsorbed on Pt(111))

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

RN 2143-61-5 HCA
CN Propyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$H_2C-CH_2-CH_3$

RN 85056-54-8 HCA
CN Propylidyne (9CI) (CA INDEX NAME)

$C-CH_2-CH_3$

IT **74-98-6P**, Propane, preparation **115-07-1P**, Propene, preparation **1333-74-0P**, **Hydrogen**, **preparation**
(surface chem. of 1-iodopropane adsorbed on Pt(111))

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

$H-H$

CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): 67
IT Bond cleavage
(carbon-**iodine**; surface chem. of 1-iodopropane adsorbed on Pt(111))
IT **115-07-1D**, Propylene, adsorbed intermediate
2143-61-5D, Propyl, adsorbed intermediate
85056-54-8D, Propylidyne, adsorbed intermediate
(surface chem. of 1-iodopropane adsorbed on Pt(111))
IT **74-98-6P**, Propane, preparation **115-07-1P**, Propene, preparation **1333-74-0P**, **Hydrogen**, **preparation** 14362-44-8P, Atomic **Iodine**, preparation
(surface chem. of 1-iodopropane adsorbed on Pt(111))

L56 ANSWER 3 OF 16 HCA
126:211755 Evidence for Divalent **Iodine** (9-I-2) Radical Intermediates in the Thermolysis of (tert-Butylperoxy)iodanes. An Unusually Efficient Deiodination of o-Iodocumyl Alcohols by Cyclohexyl Radicals. Dolenc, Darko; Plesnicar, Bozo (Department of Chemistry, University of Ljubljana, Ljubljana, 1000, Slovenia). Journal of the American Chemical Society, 119(11), 2628-2632 (English) **1997.** CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.
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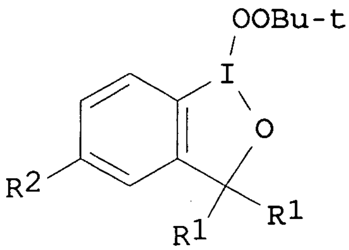


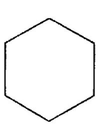
I

AB 1-(Tert-Butylperoxy)-3,3-dimethyl-1H-1,2-benziodoxoles (Ia: R1 = Me, R2 = H; Ib: R1 = Me, R2 = OMe) and 1-(tert-butylperoxy)-3,3-bis(trifluoromethyl)-5-methyl-1H-1,2-benziodoxole (Ic: R1 = CF3, R2 = Me) were prepd. from the corresponding chloroiodanes and tert-Bu hydroperoxide in the presence of potassium tert-butoxide in THF. Products, kinetic data for the decompn. of I in cyclohexane, benzene, toluene, and acetonitrile (Ea = 31.0 .+-. 1.0 kcal/mol, log A = 17.0 .+-. 0.5; 35-70.degree.), and the increased rate of decompn. of Ic in benzene-d6 in the presence of a magnetic field (7 T) indicate that homolytic cleavage of the I-O bond in I with the formation of iodanyl (9-I-2) and tert-butylperoxyl radicals is the primary decompn. step. The nearly quant. formation of iodocyclohexane during the decompn. of Ic in cyclohexane is due to the unexpected reaction of cyclohexyl radicals with 2-(2-iodo-5-methylphenyl)-1,1,1,3,3,3-hexafluoro-2-propanol, a primary decompn. product of Ic. The results of a sep. study of the deiodination of o-iodocumyl alcs. by cyclohexyl radicals are consistent with an SH2 type mechanism.

IT **110-82-7**, Cyclohexane, reactions
(cyclohexyl radical precursor with di-tert-Bu peroxyoxalate; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

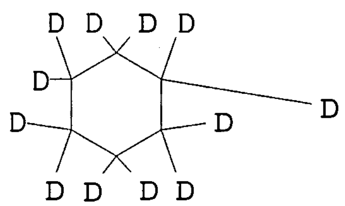
RN 110-82-7 HCA

CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT **1735-17-7**, Cyclohexane-d12
(cyclohexyl radical precursor with di-tert-Bu peroxyoxalate; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes,

and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
RN 1735-17-7 HCA
CN Cyclohexane-d12 (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)
ST divalent **iodine** radical intermediate thermolysis peroxyiodane; iodane peroxy thermolysis radical intermediate; deiodination iodocumyl alc cyclohexyl radical
IT Dehalogenation kinetics
Dehalogenation kinetics
(deiodination kinetics; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
IT Magnetic field
(effect on thermolysis kinetics; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
IT Deiodination
Thermal decomposition
Thermal decomposition kinetics
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
IT Alcohols, reactions
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
IT Reaction constant
(for deiodination; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)
IT Recombination reaction
(geminate; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes,

and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT **Hydrogen** bond
(intramol., **formation** of, enthalpy of, of o-iodocumyl alcs.; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT Hydrogen bond
Hydrogen bonding enthalpy
(intramol., of o-iodocumyl alcs.; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT Deiodination
Deiodination
(kinetics; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT Substituent effects
(on deiodination kinetics; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 1876-22-8, Di-tert-butyl peroxyoxalate
(cyclohexyl radical precursor with cyclohexane; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT **110-82-7**, Cyclohexane, reactions
(cyclohexyl radical precursor with di-tert-Bu peroxyoxalate; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT **1735-17-7**, Cyclohexane-d12
(cyclohexyl radical precursor with di-tert-Bu peroxyoxalate; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 71401-76-8
(debromination; evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 444-29-1, 2-(Trifluoromethyl)iodobenzene 610-97-9, Methyl

2-iodobenzoate 164019-56-1 187939-72-6 187939-73-7
187939-74-8 187939-75-9
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 65653-64-7P 69352-05-2P 187939-66-8P 187939-67-9P
187939-68-0P
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 187939-76-0P
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 626-62-0P, Iodocyclohexane 15619-54-2P, tert-Butyl cyclohexyl peroxide 18774-10-2P, Benzyl tert-butyl peroxide
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 75-91-2 69352-01-8 69352-04-1 187939-65-7
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

IT 93-58-3P, Methyl benzoate 98-08-8P, (Trifluoromethyl)benzene
617-94-7P 935-67-1P 2142-70-3P 71401-82-6P 187939-77-1P
(evidence for divalent **iodine** (9-I-2) radical intermediates in the thermolysis of (tert-butylperoxy)iodanes, and efficient deiodination of o-iodocumyl alcs. by cyclohexyl radicals)

L56 ANSWER 4 OF 16 HCA COPYRIGHT 2006 ACS on STN

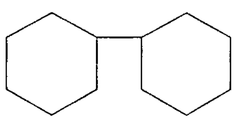
126:192814 Diffusion-Kinetic Modeling of the .gamma.-Radiolysis of Liquid Cycloalkanes. LaVerne, Jay A.; Pimblott, Simon M.; Wojnarovits, Laszlo (Radiation Laboratory, University of Notre Dame, Notre Dame, IN, 46556, USA). Journal of Physical Chemistry A, 101(8), 1628-1634 (English) **1997.** CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB A deterministic diffusion-kinetic model has been successfully applied to the radiation chem. occurring in a typical spur produced in the .gamma.-radiolysis of liq. cyclopentane, cyclohexane, and cyclooctane. The predictions of the yields of the cycloalkenes, bicycloalkyls, and the cycloalkyl iodides in solns. of **iodine** are in excellent agreement with exptl. data. The

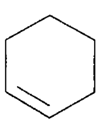
major adjustable parameters in the model are the characteristic radii of the initial Gaussian spatial distributions of the reactive species. Values for these radii were found to be 0.5, 1.1, and 0.55 nm in cyclopentane, cyclohexane, and cyclooctane, resp. The results suggest that the spurs of cyclopentane and cyclooctane are very small, ca. one mol. diam., with resulting large local concns. of reactants. With cyclohexane, the spur size is twice as large and the initial local concns. are an order of magnitude smaller. The exptl. obsd. temporal invariance of the cyclohexyl radical can be explained by competing effects in the spur evolution. Details and implications of the spur model are discussed.

IT **92-51-3**, Bicyclohexyl **110-83-8**, Cyclohexene, formation (nonpreparative) **142-29-0**, Cyclopentene **931-88-4**, Cyclooctene **1636-39-1**, Bicyclopentyl **3170-58-9**, Cyclohexyl **3889-74-5**, Cyclopentyl **4566-79-4**, Cyclooctyl **6708-17-4**, Bicyclooctyl
(deterministic diffusion-kinetic modeling of radiation chem. occurring in spurs produced in .gamma.-radiolysis of liq. cycloalkanes)

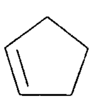
RN 92-51-3 HCA
CN 1,1'-Bicyclohexyl (9CI) (CA INDEX NAME)



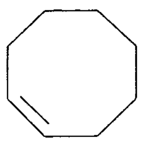
RN 110-83-8 HCA
CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



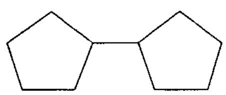
RN 142-29-0 HCA
CN Cyclopentene (8CI, 9CI) (CA INDEX NAME)



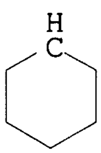
RN 931-88-4 HCA
CN Cyclooctene (8CI, 9CI) (CA INDEX NAME)



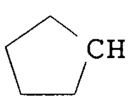
RN 1636-39-1 HCA
CN 1,1'-Bicyclopentyl (9CI) (CA INDEX NAME)



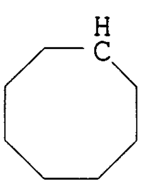
RN 3170-58-9 HCA
CN Cyclohexyl (6CI, 8CI, 9CI) (CA INDEX NAME)



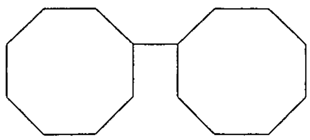
RN 3889-74-5 HCA
CN Cyclopentyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4566-79-4 HCA
CN Cyclooctyl (7CI, 8CI, 9CI) (CA INDEX NAME)

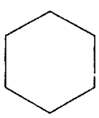


RN 6708-17-4 HCA
CN 1,1'-Bicyclooctyl (9CI) (CA INDEX NAME)

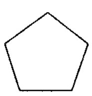


IT **110-82-7**, Cyclohexane, reactions **287-92-3**,
Cyclopentane **292-64-8**, Cyclooctane **7553-56-2**,
Iodine, reactions
(deterministic diffusion-kinetic modeling of radiation chem. occurring in spurs produced in .gamma.-radiolysis of liq. cycloalkanes)

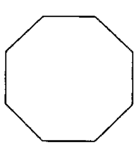
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 287-92-3 HCA
CN Cyclopentane (8CI, 9CI) (CA INDEX NAME)



RN 292-64-8 HCA
CN Cyclooctane (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **92-51-3**, Bicyclohexyl **110-83-8**, Cyclohexene,

formation (nonpreparative) **142-29-0**, Cyclopentene
626-62-0, Cyclohexyl iodide **931-88-4**, Cyclooctene
1333-74-0, **Hydrogen, formation** (nonpreparative)
1556-10-1, Cyclooctyl iodide 1556-18-9, Cyclopentyl iodide
1636-39-1, Bicyclopentyl **3170-58-9**, Cyclohexyl
3889-74-5, Cyclopentyl **4566-79-4**, Cyclooctyl
6708-17-4, Bicyclooctyl 12385-13-6, Atomic
hydrogen, formation (nonpreparative)
(deterministic diffusion-kinetic modeling of radiation chem. occurring in spurs produced in .gamma.-radiolysis of liq. cycloalkanes)

IT **110-82-7**, Cyclohexane, reactions **287-92-3**, Cyclopentane **292-64-8**, Cyclooctane **7553-56-2**, **Iodine**, reactions
(deterministic diffusion-kinetic modeling of radiation chem. occurring in spurs produced in .gamma.-radiolysis of liq. cycloalkanes)

L56 ANSWER 5 OF 16 HCA

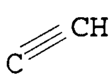
122:290187 Surface Chemistry of Chloroiodomethane, Coadsorbed with H and O, on Pt(111). Zhou, X.-L.; Liu, Z.-M.; Kiss, J.; Sloan, D. W.; White, J. M. (Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712, USA). Journal of the American Chemical Society, 117(12), 3565-92 (English) **1995**. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB Using temp. programmed desorption (TPD), predosed oxygen TPD (POTPD), high-resoln. electron energy loss spectroscopy (HREELS), and Auger electron and XPS (AES and XPS), we have investigated the chem. of chloroiodomethane (ClCH2I) dosed onto clean, D-covered and O-covered Pt(111). At or below 100 K, ClCH2I adsorbs molecularly on all these surfaces. While ClCH2I in physisorbed multilayers desorbs reversibly, a significant portion in the first monolayer dissocs. during heating. In the absence of D and O, dissocn. begins with C-I bond cleavage at .apprx.150 K. Once the C-I bond breaks, several competitive reactions take place below 260 K: (1) hydrogenation of CH2Cl(a) to form CH3Cl(g) beginning near 150 K, (2) Cl-CH2(a) bond cleavage to form Cl(a) and CH2(a) above 170 K, (3) dehydrogenation of CH2(a) to CH(a) beginning near 180 K and increasing rapidly above 200 K, (4) hydrogenation of CH2(a) to CH4(g) above 170 K, and (5) HCl and **H2 formation** and desorption above 200 K.
At 260 K, the surface species are identified as I(a), CH(a), Cl(a), and a small quantity (.apprx.0.02 ML) of CH2(a). The remaining CH2(a) reacts with itself and Cl(a) to form CH4(g), HCl(g), and CH(a) at 360 K. Cl(a) remnants react with CH(a) at 415 K, producing HCl(g) and CCH(a). The residual CH(a) fragments react at 520 K, yielding H2(g), Cx(a), and more CCH(a). Finally, dehydrogenation of CCH(a) occurs between 550 and 700 K, releasing H2 and leaving

carbon, presumably clustered. Coadsorbed D atoms weaken the bonding between ClCH2I and the surface, decrease the amt. of ClCH2I dissocg., and suppress the complete decompn. to carbon for those ClCH2I mols. that do dissoc. In TPD with coadsorbed D, besides the addn. products (i.e., CH3D, CH2D2 and CH2DCl), there are also **H**-D exchange **products** for methane (i.e., CHD3 and CD4) but not for Me chloride (i.e., no CHD2Cl and CD3Cl). Coadsorbed O atoms attenuate slightly the dissocn. of ClCH2I, but strengthen its bonding with the surface. With increasing O coverage, the yields of CH4, CH3Cl, H2, and HCl (reaction products found in the absence of O(a)) decrease; other reaction products, H2O, CO2, CO, CH2O, and CH2Cl2, appear and increase. To our knowledge, this is the first report of formaldehyde produced by the oxidn. of a CH2 precursor on Pt(111). Reaction paths are discussed, as are the effects of coadsorbed halogen atoms on hydrogenation, C-C coupling, and oxidn. of CH2.

IT **2122-48-7D**, Ethynyl radical, surface tied .eta.2- **2465-56-7D**, Methylene, surface tied **3315-37-5D**, Carbon monohydride, surface tied
(surface chem. of chloroiodomethane, coadsorbed with H and O, on Pt(111))

RN 2122-48-7 HCA
CN Ethynyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 2465-56-7 HCA
CN Methylene (8CI, 9CI) (CA INDEX NAME)

CH_2

RN 3315-37-5 HCA
CN Methylidyne (8CI, 9CI) (CA INDEX NAME)

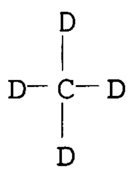
CH

IT **74-82-8P**, Methane, preparation **558-20-3P**, Tetradeuteriomethane **676-49-3P**, Deuteriomethane **676-55-1P**, Dideuteriomethane **676-80-2P**, Trideuteriomethane **1333-74-0P**, Dihydrogen, preparation
(surface chem. of chloroiodomethane, coadsorbed with H and O, on Pt(111))

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 558-20-3 HCA
CN Methane-d4 (8CI, 9CI) (CA INDEX NAME)



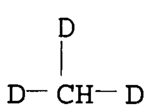
RN 676-49-3 HCA
CN Methane-d (6CI, 8CI, 9CI) (CA INDEX NAME)

$H_3C—D$

RN 676-55-1 HCA
CN Methane-d2 (6CI, 8CI, 9CI) (CA INDEX NAME)

$D—CH_2—D$

RN 676-80-2 HCA
CN Methane-d3 (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): 67
IT Bond cleavage
(carbon-**iodine**, surface chem. of chloroiodomethane, coadsorbed with H and O, on Pt(111))
IT 593-71-5, Chloroiodomethane **2122-48-7D**, Ethynyl radical, surface tied .eta.2- **2465-56-7D**, Methylene, surface tied **3315-37-5D**, Carbon monohydride, surface tied 6806-86-6D,

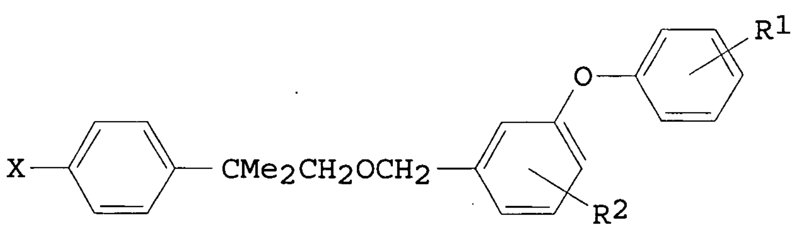
Chloromethyl, surface tied 12385-13-6, reactions 14362-44-8D, **Iodine**, atomic, surface tied, reactions 16873-17-9, Monodeuterium, reactions 17778-80-2, Monooxygen, reactions 22537-15-1D, surface tied, reactions
(surface chem. of chloroiodomethane, coadsorbed with H and O, on Pt(111))

IT 50-00-0P, Formaldehyde, preparation **74-82-8P**, Methane, preparation 74-87-3P, Methyl chloride, preparation **558-20-3P**, Tetradeuteriomethane **676-49-3P**, Deuteriomethane **676-55-1P**, Dideuteriomethane **676-80-2P**, Trideuteriomethane 1111-89-3P, Chlorotrideuteromethane **1333-74-0P**, Dihydrogen, preparation 4960-86-5P, Chlorodeuteromethane 4960-87-6P, Chlorodideuteromethane 7647-01-0P, **Hydrogen** chloride, **preparation**
(surface chem. of chloroiodomethane, coadsorbed with H and O, on Pt(111))

L56 ANSWER 6 OF 16 HCA COPYRIGHT 2006 ACS on STN

116:58945 Preparation of 3-phenoxybenzyl 2-(4-hydroxyphenyl)-2-methylpropyl ethers as intermediates for insecticides. Fukunaga, Yuji; Mita, Ryuichi; Umemoto, Mitsumasa (Kanto Chemical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 03197439 A2 **19910828** Heisei, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1989-336602 19891227.

GI

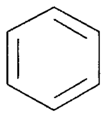


I

AB The title compds. I (R1, R2 = H, F; X = OH), useful as intermediates for insecticides and acaricides, are prepd. by treating 3-phenoxybenzyl 2-(4-halophenyl)-2-methylpropyl ethers I (X = Cl, Br, iodo) with Mg followed by O. A mixt. of Mg and **iodine** in THF was refluxed for 1 h, mixed with I (R1 = R2 = **H**, X = Br) (**prepn.** given) at .ltoreq.10.degree., refluxed for 10 h, and treated with O at room temp. for 5 h to give 93.2% I (R1 = R2 = H, X = OH).

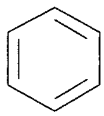
IT **71-43-2**, Benzene, reactions
(reaction of, with methallyl chloride)

RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)

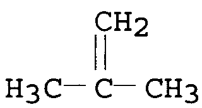


IC ICM C07C043-295
ICS C07C041-26
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
IT **71-43-2**, Benzene, reactions
(reaction of, with methallyl chloride)

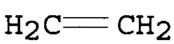
L56 ANSWER 7 OF 16 HCA COPYRIGHT 2006 ACS on STN
108:150625 Activation of benzene carbon-hydrogen bonds via photolysis or thermolysis of (.eta.5-C5Me5)2Zr(alkyl)H. Isolation of (.eta.5-C5Me5)2Zr(C6H5)H and its conversion to a complex containing a tetramethylfulvene ligand. Miller, Frederick D.; Sanner, Robert D. (Dep. Chem., Arizona State Univ., Tempe, AZ, 85287-1604, USA). Organometallics, 7(4), 818-25 (English) **1988.** CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CASREACT 108:150625.
AB A new high-yield synthesis of Cp*2ZrH2 (Cp* = .eta.5-C5Me5) is described, and olefin insertion into its Zr-H bond is used to prep. several new Cp*2Zr(alkyl)H complexes. Photolysis or thermolysis of Cp*2Zr(alkyl)H in benzene yields the resp. alkane by intramol. reductive elimination of the cis alkyl and hydride ligands, as well as the benzene C-**H** bond activation **product** Cp*2Zr(C6H5)H. Photochem. induced reductive elimination is also obsd. for Cp*2Zr(C6H5)H and Cp*2ZrH2. Deuterium-labeling expts. show that hydrogen exchange between the hydride and Cp* Me groups occurs in both Cp*2Zr(H)CH2CH(CH3)2 and Cp*2Zr(C6H5)H. An addnl. exchange process in Cp*2Zr(C6H5)H involves the hydride ligand and an ortho Ph hydrogen atom. Thermolysis of Cp*2Zr(C6H5)H in benzene causes quant. evolution of dihydrogen and reversibly forms the tetramethylfulvene complex Cp*(.eta.6-C5Me4CH2)Zr(C6H5). Reaction of this compd. with **iodine** produces the Cp* ring substituted Ph iodide Cp*(.eta.5-C5Me4CH2I)Zr(C6H5)I. Several of the transformations involving Cp*2Zr(C6H5)H are believed to proceed via .beta.-hydrogen elimination from the Ph group to yield a benzyne dihydride intermediate.
IT **71-43-2**, reactions
(photochem. reaction of, with zirconocene alkyl hydrides)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



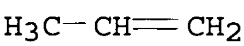
IT **115-11-7**, Isobutene, reactions
(reaction of, with zirconocene dideuteride)
RN 115-11-7 HCA
CN 1-Propene, 2-methyl- (9CI) (CA INDEX NAME)



IT **74-85-1**, Ethylene, reactions **115-07-1**, Propene, reactions
(reaction of, with zirconocene dihydride)
RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)



RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
IT **71-43-2**, reactions
(photochem. reaction of, with zirconocene alkyl hydrides)
IT 112532-20-4P
(**prepn.**, photochem. **hydrogen** exchange reaction, and thermolysis of)
IT **115-11-7**, Isobutene, reactions
(reaction of, with zirconocene dideuteride)
IT **74-85-1**, Ethylene, reactions **115-07-1**, Propene, reactions
(reaction of, with zirconocene dihydride)

L56 ANSWER 8 OF 16 HCA COPYRIGHT 2006 ACS on STN
106:102511 Isomerization of the hydridoalkylrhodium complexes formed on oxidative addition of rhodium to alkane carbon-hydrogen bonds. Evidence for the intermediacy of .eta.2-alkane complexes. Periana, Roy A.; Bergman, Robert G. (Dep. Chem., Univ. California, Berkeley,

CA, 94720, USA). Journal of the American Chemical Society, 108(23), 7332-46 (English) **1986.** CODEN: JACSAT. ISSN: 0002-7863.
OTHER SOURCES: CASREACT 106:102511.

AB The products of insertion of the coordinatively unsatd. fragment Cp*RhL (I; Cp* = .eta.5-pentamethylcyclopentadienyl, L = PMe3 throughout this abstr.) into alkane C-**H** bonds are **generated** by irradn. of Cp*(L)RhH2 (II) or thermal decompn. of Cp*(L)Rh(R)H (III; R = CH2CMe3) at <-30.degree. in alkane solvents. The products III (R = alkyl) were synthesized independently, also at low temp., from the corresponding Cp*(L)Rh(R)X (X = halo) by lithiation with Me3CLi followed by protonation. Alternatively, the highly nucleophilic complex Li[Cp*(L)RhH], prepd. by deprotonating II, gives III (R = alkyl) upon treatment with alkyl tosylates. Generating I in mixts. of linear alkanes gave only the products of insertion into primary C-H bonds, even at -100.degree.. The relative rate consts. for I formation correlate directly with the no. of secondary C-H bonds in the alkane, suggesting that insertion occurs initially into all the C-H bonds of the alkane. However, even at very low temps. the secondary-insertion products rearrange quickly and intramolecularly to the primary products, probably via .eta.2-C-H alkane complexes. These synthetic and 13C-labeled III (R = alkyl) at low temps. Warming these complexes to -80.degree. in an arom. solvent reveals isotope rearrangements which confirm that they interconvert intramolecularly at rates competitive with or in some cases faster than their reductive elimination. E.g., rearrangement of the 13C,2H-labeled III [R = Et, (1-methylcyclopropyl)methyl] showed that the I fragment migrates and inserts most rapidly into the .alpha. positions; reductive elimination is the slowest process which occurs. The kinetic isotope effect for oxidative addn. of I into the C-H bonds of hexane (detd. by competition techniques) is small [(kH/kD) = 1.1 .+-. 0.1], whereas that for reductive elimination (obtained from directly measured rates) from III (R = Et) is both large and inverse [(kH/kD) = 0.5 .+-. 0.1]. These results provide further support for the existence of intermediate .eta.2-C-H alkane complexes.

IT **74-84-0**, reactions **74-98-6**, reactions **75-19-4** **75-28-5**, Isobutane **106-97-8**, reactions **109-66-0**, reactions **110-54-3**, reactions **111-65-9**, reactions **287-23-0** **287-92-3** **1630-94-0**, 1,1-Dimethylcyclopropane
(insertion reaction of, with (pentamethylcyclopentadienyl)(trimethylphosphine)rhodium)

RN 74-84-0 HCA

CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 75-19-4 HCA
CN Cyclopropane (8CI, 9CI) (CA INDEX NAME)

RN 75-28-5 HCA
CN Propane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)

```
      CH3
      |
H3C— CH— CH3
```

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

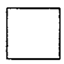
RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-Me$

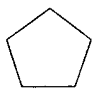
RN 111-65-9 HCA
CN Octane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_6-Me$

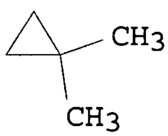
RN 287-23-0 HCA
CN Cyclobutane (6CI, 8CI, 9CI) (CA INDEX NAME)



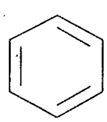
RN 287-92-3 HCA
CN Cyclopentane (8CI, 9CI) (CA INDEX NAME)



RN 1630-94-0 HCA
CN Cyclopropane, 1,1-dimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **71-43-2**, reactions **112-40-3** **124-18-5**
2037-26-5
(insertion reaction of, with (pentamethylcyclopentadienyl)(trimethylphosphine)rhodium, kinetics of)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 112-40-3 HCA
CN Dodecane (8CI, 9CI) (CA INDEX NAME)

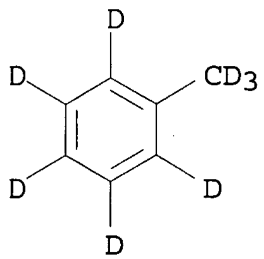
Me— $(CH_2)_{10}$—Me

RN 124-18-5 HCA
CN Decane (8CI, 9CI) (CA INDEX NAME)

Me— $(CH_2)_8$—Me

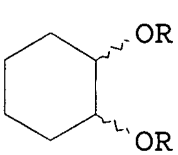
RN 2037-26-5 HCA

CN Benzene-d5, methyl-d3- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22
IT **74-84-0**, reactions **74-98-6**, reactions
75-19-4 **75-28-5**, Isobutane **106-97-8**,
reactions **109-66-0**, reactions **110-54-3**,
reactions **111-65-9**, reactions **287-23-0**
287-92-3 993-07-7, Trimethylsilane **1630-94-0**,
1,1-Dimethylcyclopropane
(insertion reaction of, with (pentamethylcyclopentadienyl)(trimethylphosphine)rhodium)
IT **71-43-2**, reactions **112-40-3** **124-18-5**
2037-26-5
(insertion reaction of, with (pentamethylcyclopentadienyl)(trimethylphosphine)rhodium, kinetics of)
IT 69178-16-1
(reaction of, with **iodine**)

L56 ANSWER 9 OF 16 HCA
94:3770 Stereoselective hydroxylation with thallium(I) acetate and **iodine**: trans- and cis-1,2-cyclohexanediols. Cambie, R. C.; Rutledge, P. S. (Dep. Chem., Univ. Auckland, Auckland, N. Z.). Organic Syntheses, 59, 169-76 (English) **1980.** CODEN: ORSYAT. ISSN: 0078-6209. OTHER SOURCES: CASREACT 94:3770.
GI


II

AB Cyclohexene (I) was refluxed with (AcO)2Tl and **iodine** in AcOH for 9 h to give trans-II (R = Ac) which was hydrolized to give 65-70% trans-II (R = OH). I was treated with (AcO)2Tl and

iodine in AcOH at 80.degree. for 5 h, and then H2O added and the mixt. refluxed 9 **h** and the **product** isolated and hydrolyzed to give 70-75% cis-II (R = OH).

IT **7553-56-2**, reactions
(reaction with thallium acetate and cyclohexene, stereoselective hydroxylation by)

RN 7553-56-2 HCA

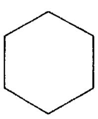
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **110-82-7**, reactions
(stereoselective hydroxylation of, by thallium acetate and **iodine**)

RN 110-82-7 HCA

CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 24-5 (Alicyclic Compounds)

IT Hydroxylation
(stereoselective, of cyclohexene by thallium acetate and **iodine**)

IT Stereochemistry
(stereoselectivity, in hydroxylation, of cyclohexene by thallium acetate and **iodine**)

IT **7553-56-2**, reactions
(reaction with thallium acetate and cyclohexene, stereoselective hydroxylation by)

IT **110-82-7**, reactions
(stereoselective hydroxylation of, by thallium acetate and **iodine**)

L56 ANSWER 10 OF 16 HCA COPYRIGHT 2006 ACS on STN

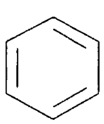
92:44068 An interpretation of the inhibition of carbon-hydrogen-oxygen flames by carbon-hydrogen-X compounds. Fristrom, R. M.; Van Tiggelen, P. (Appl. Phys. Lab., Johns Hopkins Univ., Baltimore, MD, USA). Symposium (International) on Combustion, [Proceedings], Volume Date 1978, 17, 773-85 (English) **1979.** CODEN: SYMCAQ. ISSN: 0082-0784.

AB The effectiveness of inhibitors in premixed flames can be compared using the dimensionless inhibition index .PHI.: .PHI.EXP= (V - VIn) O2/VIn. Indexes between one and forty were obsd. exptl. for

halogenated inhibitors. .PHI.EXP Appears to be an additive function of the inhibitors' at. makeup so that self-consistent at. indexes can be derived from inhibitor studies: .PHI.EXP= nH.PHI.H + nC.PHI.C + .sum.(x) nx.PHI.x. For hydrocarbon-O2 flames the reactions which dominate halogen inhibition are: radical scavenging which changes reactive radicals into unreactive radicals or mols., and halogen atom-assisted cyclic recombination of inactive radicals H + X + M = HX + M.bul. followed by HX + (H, O, OH) = X + (H2,OH,H2). A simple flame model allows the exptl. at. halogen indexes to be interpreted in terms of elementary inhibitor reactions: .PHI.x = (Nx + M.bul.kx/.vector.k)KF. The scavenging term, Nx, is either 1 or 2 depending on the group to which the halogen atom is bound in the inhibitor mol., while the recombination term depends on the chain length as controlled by the ratio of radical recombination (H + X + M = HX + M.bul.) to **prodn.** (**H** + O2 = OH + O).
Thus, the prediction of the inhibition index for a halogenated compd. in any hydrocarbon-O2 flame requires only a knowledge of the recombination rate consts. for Cl, Br, and I atoms. The recombination rate for F is low compared with the scavenging contribution. C and H contributions to the index are small. They are additive and can be evaluated from the data or from the burning velocity curve of the uninhibited flame.

IT **71-43-2**, reactions **74-85-1**, reactions
74-86-2, reactions **74-98-6**, reactions
110-54-3, reactions
(flames, halogen inhibitors for)

RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 74-86-2 HCA
CN Ethyne (9CI) (CA INDEX NAME)

$HC{\equiv}CH$

RN 74-98-6 HCA

CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-Me$

IT **7553-56-2**, uses and miscellaneous
(hydrocarbon flame inhibitors)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 50-1 (Propellants and Explosives)
IT **71-43-2**, reactions **74-85-1**, reactions
74-86-2, reactions **74-98-6**, reactions
110-54-3, reactions
(flames, halogen inhibitors for)
IT **7553-56-2**, uses and miscellaneous 7726-95-6, uses and miscellaneous 7782-41-4, uses and miscellaneous 7782-50-5, uses and miscellaneous
(hydrocarbon flame inhibitors)

L56 ANSWER 11 OF 16 HCA
88:14226 Temperature dependence of product yields from the liquid phase radiolysis of n-hexane. Avdonina, E. N.; Lebedev, V. A. (Mosk. Gos. Univ., Moscow, USSR). Khimiya Vysokikh Energii, 11(4), 376 (Russian) **1977.** CODEN: KHVKAO. ISSN: 0023-1193.
AB The radiolysis of hexane with and without the addn. of I in the temp. range of -80 to 150.degree. was studied. The following processes were detected upon an increase in the temp.: the yields of formation of hexenes and olefins do not change; the amt. of polymeric products increases; and primary destruction of hexane with the **formation** of reactive **H** atoms and radicals also increases. The disproportionation of radicals decreases and the recombination of radicals increases as the temp. increases.
IT **1333-74-0P**, preparation **25264-93-1P**
(formation of, from radiolysis of hexane in liq. phase, temp. dependence of yields of)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

RN 25264-93-1 HCA
CN Hexene (8CI, 9CI) (CA INDEX NAME)

CM 1

CRN 110-54-3
CMF C6 H14

Me—$(CH_2)_4$—Me

IT **7553-56-2**, uses and miscellaneous
(radiolysis of liq. hexane contg., temp. dependence of product yields from)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

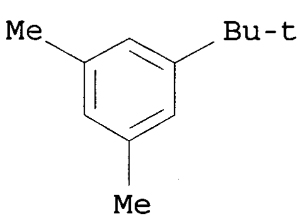
IT **110-54-3**, reactions
(radiolysis of, in liq. phase, temp. dependence of product yields from)
RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

Me—$(CH_2)_4$—Me

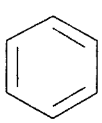
CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **1333-74-0P**, preparation **25264-93-1P**
(formation of, from radiolysis of hexane in liq. phase, temp. dependence of yields of)
IT **7553-56-2**, uses and miscellaneous
(radiolysis of liq. hexane contg., temp. dependence of product yields from)
IT **110-54-3**, reactions
(radiolysis of, in liq. phase, temp. dependence of product yields from)

L56 ANSWER 12 OF 16 HCA COPYRIGHT 2006 ACS on STN
82:16528 2,6-Dimethylchlorobenzene. Goto, Ryozo; Maruyama, Kazuhiro; Konami, Tsugio (Kuraray Co., Ltd.). Jpn. Tokkyo Koho JP 49013773 B4 **19740403** Showa, 3 pp. (Japanese). CODEN: JAXXAD.

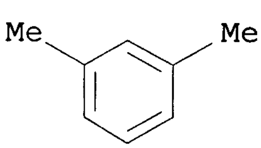
APPLICATION: JP 1968-45486 19680628.
GI For diagram(s), see printed CA Issue.
AB 2,6-Dimethylchlorobenzene (I; R = Cl, R1 = R2 = **H**) (II) was **prepd.** by transalkylation of I (R = Cl, R1 = H, R2 = Me3C) (III), obtained from chlorination of I (R = R1 = H, R2 = Me3C) (IV) in the presence of a Lewis acid or **iodine**, with m-xylene, PhMe, or C6H6 in the presence of anhyd. AlCl3, TiCl4, SnCl4, H3PO4 or solid H3PO4 or HBF4. Thus, IV, obtained from reaction of m-xylene with Me2C:CH2, was chlorinated in the presence of **iodine** to give 72% III and 28% by-**product** (I; R = **H**, R1 = Cl, R2 = Me3C). III was treated with m-xylene in the presence of anhyd. AlCl3 45 min at room temp. and fractionally distd. to give 90% II and 66% IV.
IT **98-19-1P**
(prepn. and chlorination of)
RN 98-19-1 HCA
CN Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)



IT **71-43-2**, reactions **108-38-3**, reactions
(transalkylation of)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 108-38-3 HCA
CN Benzene, 1,3-dimethyl- (9CI) (CA INDEX NAME)

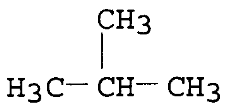


IC C07C; B01J
CC 25-3 (Noncondensed Aromatic Compounds)

IT **98-19-1P**
(prepn. and chlorination of)
IT **71-43-2**, reactions **108-38-3**, reactions
(transalkylation of)

L56 ANSWER 13 OF 16 HCA COPYRIGHT 2006 ACS on STN
75:34685 Electron spin resonance study of the rate constants for reaction of hydrogen atoms with organic compounds in aqueous solution. Schuler, Robert H.; Neta, P.; Fessenden, Richard W. (Mellon Inst. Sci., Carnegie-Mellon Univ., Pittsburgh, PA, USA). Journal of Physical Chemistry, 75(11), 1654-66 (English) **1971.** CODEN: JPCHAX. ISSN: 0022-3654.
AB **H** atoms **produced** by the electron-proton neutralization reaction in aq. soln. show abnormal ESR lines because of an initial nonequil. population of the 4 possible electron-nuclear spin levels. The high-field line is obsd. in enhanced absorption and the low-field line in emission. At the normal power levels employed in these ESR expts. relaxation to an equil. distribution occurs with a period .apprx.50 .mu.sec and chem. reactions will effectively compete with this relaxation if solutes are present at concns. such that the pseudo-1st-order rate const. ks[S] is >104 sec-1. A steady-state ESR method for detg. the rate consts. for reaction of H atoms with added solutes was developed which is based on this competition. The effect of exptl. variables on the obsd. signal intensity is examd. and in particular it is noted that the effect of power on the competitive situation is completely in accord with the proposed model. In cases where comparative data by this and other methods are available relative rate consts. are, in most cases, in good agreement. The abs. scale is established by internal comparison with solutes having known rate consts. Observations on >60 compds. with 2nd-order rate consts. ranging from 105 to 109M-1 sec-1 were carried out. For satd. aliphatic compds. the rate consts. increase with mol. size, being .apprx.105M-1 sec-1 or less only for the simplest of species. A plateau level .apprx.108M-1 sec-1 is approached for aliphatic derivs. in the C6 region. As expected, mols. contg. reactive features such as double bonds, aromatic rings, or **iodine** atoms exhibit rate consts. in the region near the diffusion controlled limit.
IT **75-19-4 75-28-5 109-66-0**
287-92-3
(reaction of, with atomic hydrogen)
RN 75-19-4 HCA
CN Cyclopropane (8CI, 9CI) (CA INDEX NAME)

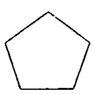
RN 75-28-5 HCA
CN Propane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

RN 287-92-3 HCA
CN Cyclopentane (8CI, 9CI) (CA INDEX NAME)



IT **74-84-0**, reactions **74-85-1**, reactions **74-98-6**, reactions **106-97-8**, reactions **110-54-3**, reactions **110-82-7**, reactions
(with atomic hydrogen, kinetics of)
RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

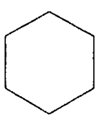
RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-Me$

RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)

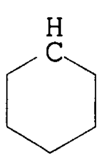


CC 22 (Physical Organic Chemistry)
IT 60-35-5 62-57-7 74-87-3 74-88-4 74-96-4 75-00-3 75-09-2 **75-19-4** **75-28-5** 75-52-5 75-65-0 75-69-4 75-84-3 78-82-0 78-83-1 78-92-2 79-08-3 79-31-2 97-69-8 107-12-0 107-95-9 **109-66-0** 111-27-3 **287-92-3** 372-09-8 543-24-8 554-95-0
(reaction of, with atomic hydrogen)
IT 50-21-5, reactions 56-23-5, reactions 56-40-6, reactions 56-41-7, reactions 57-13-6, reactions 60-29-7, reactions 64-17-5, reactions 64-18-6, reactions 64-19-7, reactions 65-85-0, reactions 67-56-1, reactions 67-63-0, reactions 67-64-1, reactions 67-66-3, reactions 71-23-8, reactions 71-36-3, reactions **74-84-0**, reactions **74-85-1**, reactions **74-98-6**, reactions 75-05-8, reactions 75-07-0, reactions 79-09-4, reactions 79-14-1, reactions **106-97-8**, reactions 107-21-1, reactions 107-92-6, reactions 109-99-9, reactions 110-15-6, reactions **110-54-3**, reactions **110-82-7**, reactions 123-91-1, reactions 141-82-2, reactions 142-62-1, reactions 144-62-7, reactions 526-83-0, reactions
(with atomic hydrogen, kinetics of)

L56 ANSWER 14 OF 16 HCA
73:135899 Effect of ion and radical scavengers on the cyclohexyl radical yield in the radiolysis of cyclohexane. Bansal, Krishan M.; Schuler, Robert H. (Mellon Inst. Radiat. Res. Lab., Carnegie-Mellon Univ., Pittsburgh, PA, USA). Journal of Physical Chemistry, 74(22), 3924-32 (English) **1970.** CODEN: JPCHAX. ISSN: 0022-3654.
AB Scavenging studies with I indicate that the yield of cyclohexyl radicals produced in the radiolysis of pure cyclohexane is

.apprx.5.7; I concns. in the range of 10-2M, however, reduce the obsd. yield to .apprx.4.2. This decrease is interpreted as being **produced** both by **H** atom and by pos. ion scavenging reactions of I. The effect of a no. of other solutes on the production of cyclohexyl radicals has also been examd. Cyclopropane reduces the yield by an amt. approx. equal to the yield of the pos. ion reactions. Ethylene has a similar effect with a superimposed redn. which results from H atom scavenging. The various electron scavengers examd. (MeBr, MeI, MeCl, SF6, N2O, and CO2) have differing effects which depend on the relative importance of secondary abstraction reactions. The comparison of MeBr and MeCl is particularly interesting because the 1st solute causes a redn. approx. equal to the yield of electron capture while the 2nd has essentially no effect. N2O is unique in that an increase is obsd. in G(C6H11.bul.) which is equal to the yield of electrons captured by the N2O. The quant. aspects of the various effects can be correlated quite well by expressions derived from a description of the concn. dependence of ionic processes in these systems if it is assumed that on the av. 1 cyclohexyl radical is produced for each neutralization that occurs between a pos. ion-electron geminate pair. The interpretation of the data is, however, more complex than in the case of **H production** because certain processes produce several cyclohexyl radicals while others produce none.

IT **3170-58-9P**
(formation of, in radiolysis of liq. cyclohexane)
RN 3170-58-9 HCA
CN Cyclohexyl (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **74-85-1**, uses and miscellaneous **75-19-4**
7553-56-2, uses and miscellaneous
(radiolysis of cyclohexane in presence of, cyclohexyl radical formation in)
RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

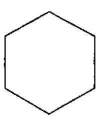
$H_2C{=}CH_2$

RN 75-19-4 HCA
CN Cyclopropane (8CI, 9CI) (CA INDEX NAME)

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

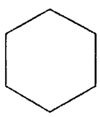
IT **110-82-7**, reactions
(radiolysis of liq., scavenger effect on cyclohexyl radical formation in)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



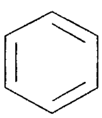
CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **3170-58-9P**
(formation of, in radiolysis of liq. cyclohexane)
IT 74-83-9 **74-85-1**, uses and miscellaneous **75-19-4**
7553-56-2, uses and miscellaneous 10024-97-2, uses and miscellaneous
(radiolysis of cyclohexane in presence of, cyclohexyl radical formation in)
IT **110-82-7**, reactions
(radiolysis of liq., scavenger effect on cyclohexyl radical formation in)

L56 ANSWER 15 OF 16 HCA COPYRIGHT 2006 ACS on STN
73:55462 Effect of concentration on the yield of hydrogen during .gamma.-radiolysis of a mixture of cyclohexane with benzene. Avdonina, E. N. (Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR). Khimiya Vysokikh Energii, 4(3), 226-8 (Russian) **1970.** CODEN: KHVKAO. ISSN: 0023-1193.
AB The yield of mol. H during .gamma.-radiolysis of cyclohexane (I)-benzene (II) mixt. depends strongly on the mixt. compn. Mol. **H** is **formed** either via a mol. mechanism in which one mol. of H is eliminated from one mol. of I, or by the interaction of H atoms with I. The reactive intermediates are, in the former case, easily quenched by II, whereas those in the latter case are not influenced. In **pure I**, the G value for H-abstraction from I by "hot" H atoms is .apprx.1.15 and that

for mol. elimination is 2.6.
IT **110-82-7**, reactions
(mixt. with benzene, radiolysis of, by gamma rays)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT **71-43-2**, reactions
(mixt. with cyclohexane, radiolysis of, by gamma rays)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



CC 22 (Physical Organic Chemistry)
IT **110-82-7**, reactions
(mixt. with benzene, radiolysis of, by gamma rays)
IT **71-43-2**, reactions
(mixt. with cyclohexane, radiolysis of, by gamma rays)

67:27551 Yield of thermal ethyl radicals from the radiolysis of ethylene-cyclohexane solutions. McCrumb, J. L.; Schuler, Robert H. (Mellon Inst., Pittsburgh, PA, USA). Journal of Physical Chemistry, 71(6), 1953-5 (English) **1967.** CODEN: JPCHAX. ISSN: 0022-3654.
AB Dil. **I2** was used to totally scavenge product Et radicals to give a measure of the concn. dependence of the abs. yield for their formation. The procedure was previously described (CA 58: 13334b). Samples which contained a known concn. of ethylene and .apprx.10-4M 131I of known relative sp. activity were outgassed and irradiated in a 60Co source to a dose of 5 .times. 17 ev./g. Approx. 25% of the **I2** reacted. The sample (0.5 ml.) was chromatographed, the EtI fraction collected, and the total activity of the fraction detd. The EtI seemed to be formed by addn. of thermal H atoms to the C2H4 and then the Et radicals by scavenging. A plot of 1/G(C2H5I*) vs. 1/[C2H4] showed an excellent linear relation which indicated that the data were in accord with simple competition between H.bul. + RH .fwdarw. H2 + R.bul. and H.bul. +

C2H4 .fwdarw. C2H5.bul. (Holroyd, CA 65: 198g). A multiplication of the measured Et radical yield by the ratios of G(cyclo-C6H11)/G(C2H5) (cf. H., loc. cit.), gives a const. total yield of C2 and C6 radicals. The **H production** can not be strongly dependent on the ethylene concn. in this range. The estd. radical yields were tabulated. The rate const. ratio gave a scavenging efficiency of 24% at 10 mM ethylene. H seemed to be produced from cyclohexane.

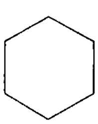
IT **2025-56-1P**
(formation of, in radiolysis of ethylene-cyclohexane solns.)
RN 2025-56-1 HCA
CN Ethyl (8CI, 9CI) (CA INDEX NAME)

H_2C-CH_3

IT **74-85-1**, reactions
(radiolysis of cyclohexane and, ethyl radical formation in)
RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

IT **110-82-7**, reactions
(radiolysis of ethylene and, ethyl radical formation in)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **2025-56-1P**
(formation of, in radiolysis of ethylene-cyclohexane solns.)
IT **74-85-1**, reactions
(radiolysis of cyclohexane and, ethyl radical formation in)
IT **110-82-7**, reactions
(radiolysis of ethylene and, ethyl radical formation in)

=> d l57 1-32 cbib abs hitstr hitind

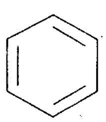
L57 ANSWER 1 OF 32 HCA
133:357158 The effect of anti-inhibition of radiolytic **hydrogen**

formation in liquids. Byakov, V. M.; Stepanov, S. V.; Stepanova, O. P. (Institute of Theoretical and Experimental Physics, Moscow, 117218, Russia). High Energy Chemistry (Translation of Khimiya Vysokikh Energii), 34(5), 284-289 (English) **2000.** CODEN: HIECAP. ISSN: 0018-1439. Publisher: MAIK Nauka/Interperiodica Publishing.

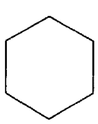
AB Anti-inhibition effect known in positronium chem. is also obsd. in the radiolysis of liqs. In particular, the yield of radiolytic **hydrogen formation** in **cyclohexane** in the presence of mol. **iodine** increased when benzene was added to a **cyclohexane** soln. This effect was rationalized on the basis of the previously advanced idea on the similarity between the formation mechanisms of positronium and radiolytic hydrogen. The assumption that the enhancement of radiolytic hydrogen yield in the aq. nitrate or nitrite solns. took place upon addn. of Mn2+, Co2+, Zn2+, etc. was also the manifestation of the anti-inhibition effect, which was known neither for positronium nor for radiolytic hydrogen in polar media, was substantiated.

IT **71-43-2**, Benzene, processes **110-82-7**, **Cyclohexane**, processes **7553-56-2**, **Iodine**, processes
(effect of anti-inhibition in radiolytic **hydrogen formation** in liqs.)

RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and

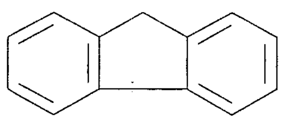
Other Reprographic Processes)
ST antiinhibition effect radiolytic **hydrogen** positronium **formation** mechanism liq; radiolysis liq hydrogen fromation mechanism antiinhibition effect
IT Radical ions
(cations; effect of anti-inhibition in radiolytic **hydrogen formation** in liqs.)
IT Radiolysis
(effect of anti-inhibition in radiolytic **hydrogen formation** in liqs.)
IT **71-43-2**, Benzene, processes **110-82-7**, **Cyclohexane**, processes 1333-74-0, Hydrogen, processes **7553-56-2**, **Iodine**, processes 7632-00-0, Sodium nitrite 7732-18-5, Water, processes 7757-79-1, Potassium nitrate, processes 14280-50-3, Lead(2+), processes 14701-22-5, Nickel(2+), processes 15158-11-9, Copper(2+), processes 16397-91-4, Manganese(2+), processes 22537-48-0, Cadmium(2+), processes 22541-53-3, Cobalt(2+), processes 23713-49-7, Zinc(2+), processes
(effect of anti-inhibition in radiolytic **hydrogen formation** in liqs.)

L57 ANSWER 2 OF 32 HCA COPYRIGHT 2006 ACS on STN
125:194845 Hypervalent (tert-Butylperoxy)iodanes Generate **Iodine** -Centered Radicals at Room Temperature in Solution: Oxidation and Deprotection of Benzyl and Allyl Ethers, and Evidence for Generation of .alpha.-Oxy Carbon Radicals. Ochiai, Masahito; Ito, Takao; Takahashi, Hideo; Nakanishi, Akinobu; Toyonari, Mika; Sueda, Takuya; Goto, Satoru; Shiro, Motoo (Faculty of Pharmaceutical Sciences, University of Tokushima, Tokushima, 770, Japan). Journal of the American Chemical Society, 118(33), 7716-7730 (English) **1996** . CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.
AB 1-(Tert-Butylperoxy)-1,2-benziodoxol-3(1H)-one (I) oxidizes benzyl and allyl ethers to the esters at room temp. in benzene or **cyclohexane** in the presence of alkali metal carbonates. Since this reaction is compatible with other protecting groups such as MOM, THP, and TBDMS ethers, and acetoxy groups, and because esters are readily hydrolyzed under basic conditions, this new method provides a convenient and effective alternative to the usual reductive deprotection. Oxidn. with I occurs readily with C-H bonds activated by both enthalpic effects (benzylic, allylic, and propargylic C-H bonds) and/or polar effects (.alpha.-oxy C-**H** bonds), **generating** .alpha.-oxy carbon-centered radicals, which can be detected by nitroxyl radical trapping. Measurement of the relative rates of oxidn. for a series of ring-substituted benzyl Bu ethers indicated that electron-releasing groups such as p-MeO and p-Me groups increase the rate of oxidn., and Hammett correlation of

the relative rate factors with the .sigma.+ consts. of substituents afforded the reaction const. .rho.+ = -0.30. The large value of the isotope effect obtained for the oxidn. of benzyl Bu ether 2d (kH/kD = 12-14) indicates that the rate-detg. step of the reactions probably involves a high degree of benzylic C-H bond breaking. The effects of mol. dioxygen were examd., and the mechanism involving the intermediacy of a tert-butylperoxy acetal and/or a hydroperoxy acetal is proposed. Particularly noteworthy is the finding that (tert-butylperoxy)iodane I can generate the tert-butylperoxy radical and an **iodine**-centered radical , even at room temp. in soln., via homolytic bond cleavage of the hypervalent **iodine** (III)-peroxy bond.

IT **86-73-7**, Fluorene **101-81-5**, Diphenylmethane **119-64-2**, Tetrahydronaphthalene **496-11-7**, Indan **613-31-0**, 9,10-Dihydroanthracene **1077-16-3**, Hexylbenzene
(oxidn. of hydrocarbons with butylperoxybenziodoxolone)

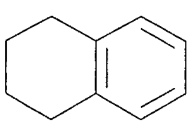
RN 86-73-7 HCA
CN 9H-Fluorene (9CI) (CA INDEX NAME)



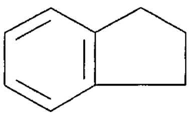
RN 101-81-5 HCA
CN Benzene, 1,1'-methylenebis- (9CI) (CA INDEX NAME)

Ph— CH_2 — Ph

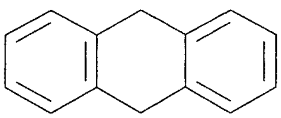
RN 119-64-2 HCA
CN Naphthalene, 1,2,3,4-tetrahydro- (8CI, 9CI) (CA INDEX NAME)



RN 496-11-7 HCA
CN 1H-Indene, 2,3-dihydro- (9CI) (CA INDEX NAME)



RN 613-31-0 HCA
CN Anthracene, 9,10-dihydro- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1077-16-3 HCA
CN Benzene, hexyl- (9CI) (CA INDEX NAME)

$Me-(CH_2)_5-Ph$

CC 22-7 (Physical Organic Chemistry)
IT Isotope effect
(deuterium; oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)
IT Kinetics of oxidation
Oxidation
Reaction constant
Solvent effect
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)
IT Ethers, reactions
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)
IT Linear free energy relationship
(Dimroth-Reichardt, oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)
IT Carboxylic acids, preparation
(esters, oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)
IT 180477-35-4P
(intermediate; oxidn. of benzyl and allyl ethers to esters by

(butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 7782-39-0, Deuterium, properties
(isotope effect; oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 29336-70-7 180477-57-0 180477-58-1
(oxidn. of alkynyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 19434-11-8P 180477-59-2P 180477-60-5P
(oxidn. of alkynyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 1829-25-0P 180477-36-5P 180477-67-2P
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 588-67-0, Benzyl butyl ether 5333-52-8, p-Methoxybenzyl butyl ether 91763-46-1, p-Methylbenzyl butyl ether 101005-09-8, Butyl m-chlorobenzyl ether 101005-10-1, Butyl p-chlorobenzyl ether
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 493-05-0, 1H-2-Benzopyran, 3,4-dihydro- 496-14-0 538-86-3, Benzyl methyl ether 539-30-0, Benzyl ethyl ether 937-54-2, Benzyl isopropyl ether 940-44-3, Benzyl sec-butyl ether 946-80-5 2040-37-1 3295-96-3 3459-80-1, Benzyl tert-butyl ether 14289-65-7 16224-09-2, Benzyl cyclohexyl ether 24806-16-4 40843-99-0, Benzyl cyclopentyl ether 50638-95-4 67528-21-6 70388-33-9 96124-85-5 135394-83-1 136375-73-0 180477-33-2, Benzyl 1-methylcyclohexyl ether 180477-34-3 180477-37-6 180477-38-7 180477-39-8 180477-40-1 180477-41-2 180477-42-3 180477-43-4 180477-44-5 180477-51-4 180477-52-5 180477-53-6 180477-54-7 180477-55-8 180477-61-6 180477-65-0 180477-68-3
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 463-79-6D, Carbonic acid, alkali metal salts 2564-83-2, TEMPO 142260-70-6, 1-(tert-Butylperoxy)-1,2-benziodoxol-3(1H)-one
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT 87-41-2P, 1(3H)-Isobenzofuranone 93-58-3P, Methyl benzoate 93-89-0P, Ethyl benzoate 93-99-2P 136-60-7P, Benzoic acid, butyl ester 774-65-2P, tert-Butyl benzoate 939-48-0P, Isopropyl benzoate 2156-96-9P 2412-73-9P, Cyclohexyl benzoate 3179-47-3P 3306-36-3P, sec-Butyl benzoate 3530-36-7P 4702-34-5P,

1H-2-Benzopyran-1-one, 3,4-dihydro- 4835-96-5P 6284-35-1P
6946-35-6P 13358-49-1P 13633-88-0P 15867-50-2P 18203-32-2P
19277-56-6P 27942-64-9P 32651-38-0P, Cyclopentyl benzoate
33693-85-5P, 1-Methylcyclohexyl benzoate 42078-65-9P 47701-93-9P
56500-46-0P 62934-33-2P 63987-54-2P 111902-22-8P
121601-93-2P 170303-74-9P 170800-84-7P 180477-45-6P
180477-46-7P 180477-47-8P 180477-48-9P 180477-49-0P
180477-50-3P 180477-56-9P 180477-62-7P 180477-63-8P
180477-64-9P 180477-66-1P 180477-69-4P 180477-70-7P
180477-71-8P 180477-72-9P
(oxidn. of benzyl and allyl ethers to esters by (butylperoxy)benziodoxolone at room temp. in benzene or **cyclohexane** in presence of alkali metal carbonate)

IT **86-73-7**, Fluorene 90-44-8, Anthrone 92-83-1, Xanthene
101-81-5, Diphenylmethane **119-64-2**,
Tetrahydronaphthalene **496-11-7**, Indan **613-31-0**,
9,10-Dihydroanthracene **1077-16-3**, Hexylbenzene
5111-69-3, 5-Methoxyindan
(oxidn. of hydrocarbons with butylperoxybenziodoxolone)

L57 ANSWER 3 OF 32 HCA COPYRIGHT 2006 ACS on STN

123:183180 Radical Reactions in the Radiolysis of Cyclopentane. Wojnarovits, Laszlo; LaVerne, Jay A. (Radiation Laboratory, University of Notre, Dame Notre Dame, IN, 46556, USA). Journal of Physical Chemistry, 99(10), 3168-72 (English) **1995.** CODEN: JPCHAX. ISSN: 0022-3654. Publisher: American Chemical Society.

AB The end products produced in the .gamma.-radiolysis of cyclopentane have been measured at very low total doses (25-50 krad). **Iodine** scavenging techniques in solns. of 0.1-30 mM were used to elucidate radical yields and reaction mechanisms. The yields of the main radical species were found to be as follows: cyclopentyl, 4.9; 1-pentyl, 0.2; 3-cyclopentenyl, 0.07; H atom, 1.3 radical/100 eV. The change in yields from neat cyclopentane to 0.1 mM **iodine** soln. suggests that about 79% of the cyclopentyl radicals escape the spur and react in the bulk medium with a disproportionation to combination ratio of 0.97. Radical precursors account for about 50% of the total end product yield, which is much smaller than found in the radiolysis of **cyclohexane** or cyclooctane. The radiolysis mechanism for cyclopentane is discussed and compared to those for **cyclohexane** and cyclooctane.

IT **109-66-0**, n-Pentane, formation (nonpreparative)
109-67-1, 1-Pentene **142-29-0**, Cyclopentene
2672-01-7, 1-Pentyl **3741-00-2**,
n-Pentylcyclopentane **29031-91-2**, Cyclopentylcyclopentene
(radical reactions in radiolysis of cyclopentane)

RN 109-66-0 HCA

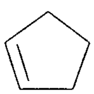
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

RN 109-67-1 HCA
CN 1-Pentene (7CI, 8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH{=}CH_2$

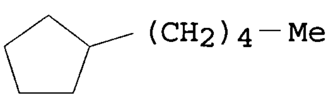
RN 142-29-0 HCA
CN Cyclopentene (8CI, 9CI) (CA INDEX NAME)



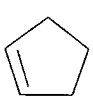
RN 2672-01-7 HCA
CN Pentyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

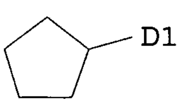
$H_2C-CH_2-CH_2-CH_2-CH_3$

RN 3741-00-2 HCA
CN Cyclopentane, pentyl- (9CI) (CA INDEX NAME)



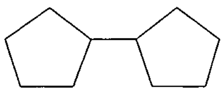
RN 29031-91-2 HCA
CN Cyclopentene, cyclopentyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



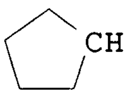


IT **1636-39-1**, Bicyclopentyl **3889-74-5**, Cyclopentyl
10577-65-8, 3-Cyclopentenyl
(radical reactions in radiolysis of cyclopentane)

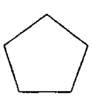
RN 1636-39-1 HCA
CN 1,1'-Bicyclopentyl (9CI) (CA INDEX NAME)



RN 3889-74-5 HCA
CN Cyclopentyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 10577-65-8 HCA
CN 2-Cyclopenten-1-yl (7CI, 8CI, 9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **287-92-3**, Cyclopentane
(radical reactions in radiolysis of cyclopentane)
RN 287-92-3 HCA
CN Cyclopentane (8CI, 9CI) (CA INDEX NAME)



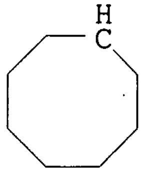
IT **7553-56-2, Iodine**, reactions
(scavenger; radical reactions in radiolysis of cyclopentane)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **109-66-0**, n-Pentane, formation (nonpreparative)
109-67-1, 1-Pentene **142-29-0**, Cyclopentene
628-17-1, n-Pentyl iodide 1333-74-0, **Hydrogen, formation** (nonpreparative) 1556-18-9, Cyclopentyl iodide
2672-01-7, 1-Pentyl **3741-00-2**,
n-Pentylcyclopentane **29031-91-2**, Cyclopentylcyclopentene
(radical reactions in radiolysis of cyclopentane)
IT **1636-39-1**, Bicyclopentyl **3889-74-5**, Cyclopentyl
10577-65-8, 3-Cyclopentenyl 12385-13-6, Atomic hydrogen,

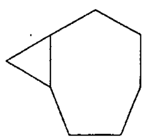
reactions
(radical reactions in radiolysis of cyclopentane)
IT **287-92-3**, Cyclopentane
(radical reactions in radiolysis of cyclopentane)
IT **7553-56-2**, **Iodine**, reactions
(scavenger; radical reactions in radiolysis of cyclopentane)

L57 ANSWER 4 OF 32 HCA COPYRIGHT 2006 ACS on STN
121:121546 Radiolysis of Cyclooctane with .gamma.-Rays and Helium Ions.
Wojnarovits, Laszlo; LaVerne, Jay A. (Radiation Laboratory, University of Notre Dame, Notre Dame, IN, 46556, USA). Journal of Physical Chemistry, 98(33), 8014-18 (English) **1994.**
CODEN: JPCHAX. ISSN: 0022-3654.
AB **Iodine** scavenging techniques have been used to examine the role of the cyclooctyl radical in the radiolysis of cyclooctane with .gamma.-rays and with 5-20-MeV helium ions. In .gamma.-radiolysis about 70% of the total yield of 6.6 cyclooctyl radicals/100 eV are scavenged with 10-4 M **iodine**, which agrees well with other studies on cycloalkanes that show most of the radicals produced in these systems react in the bulk medium at times longer than 1 ms. However, it is found that 2.5 radicals/100 eV (38%) are **produced** by **H** atom precursors as compared to a value of 1.5 cyclohexyl radicals/100 eV (25%) in **cyclohexane** . With 10-MeV helium ions (av. LET of 106 eV/nm), only 8% of the cyclooctyl radicals survive longer than a few microseconds due to the increased initial radical concn. in the helium ion track. The yield of the cross-bridged product bicyclo[3.3.0]octane (pentalane) was found to be independent of **iodine** concn. up to 0.03 M with both types of radiation. However, the pentalane yield found with 10-MeV helium ions was only one-third of that found in .gamma.-radiolysis. The most likely reason for this result is the decreased yield of singlet-state formation due to the enhanced probability of cross combination reactions of electron-cation pairs in the high-d. region of the helium ion track.
IT **4566-79-4P**, Cyclooctyl
(formation and processes of, in radiolysis of cyclooctane with gamma-rays and helium ions)
RN 4566-79-4 HCA
CN Cyclooctyl (7CI, 8CI, 9CI) (CA INDEX NAME)

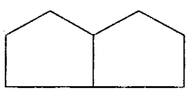


IT **286-43-1P**, Bicyclo[5.1.0]octane **694-72-4P**,

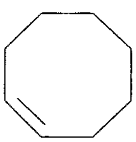
Bicyclo[3.3.0]octane **931-88-4P**, Cyclooctene
6708-17-4P, Bicyclooctyl
(formation of, in radiolysis of cyclooctane with gamma-rays and helium ions)
RN 286-43-1 HCA
CN Bicyclo[5.1.0]octane (7CI, 8CI, 9CI) (CA INDEX NAME)



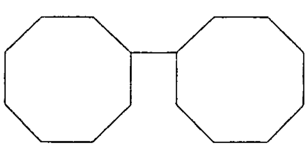
RN 694-72-4 HCA
CN Pentalene, octahydro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 931-88-4 HCA
CN Cyclooctene (8CI, 9CI) (CA INDEX NAME)



RN 6708-17-4 HCA
CN 1,1'-Bicyclooctyl (9CI) (CA INDEX NAME)

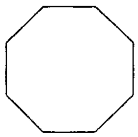


IT **7553-56-2**, **Iodine**, reactions
(radiolysis of cyclooctane and, with gamma-rays and helium ions)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **292-64-8**, Cyclooctane

(radiolysis of, with gamma-rays and helium ions, role of cyclooctyl radical in)
RN 292-64-8 HCA
CN Cyclooctane (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **4566-79-4P**, Cyclooctyl
(formation and processes of, in radiolysis of cyclooctane with gamma-rays and helium ions)
IT **286-43-1P**, Bicyclo[5.1.0]octane **694-72-4P**, Bicyclo[3.3.0]octane **931-88-4P**, Cyclooctene **6708-17-4P**, Bicyclooctyl
(formation of, in radiolysis of cyclooctane with gamma-rays and helium ions)
IT 1556-10-1P, Cyclooctyl iodide
(formation of, in radiolysis of cyclooctanewith **iodine**, with gamma-rays and helium ions)
IT **7553-56-2**, **Iodine**, reactions
(radiolysis of cyclooctane and, with gamma-rays and helium ions)
IT **292-64-8**, Cyclooctane
(radiolysis of, with gamma-rays and helium ions, role of cyclooctyl radical in)

L57 ANSWER 5 OF 32 HCA COPYRIGHT 2006 ACS on STN
112:197880 Process for preparing polyalkyltetrahydronaphthalenes. Frank, Walter C. (Union Camp Corp., USA). U.S. US 4877913 A **19891031**, 12 pp. (English). CODEN: USXXAM. APPLICATION: US 1989-303355 19890127.
AB The process for producing the title compds., comprises cycloaddn. of a substituted **C6H6** in which the substituent(s) does not interfere with a Friedel-Crafts type alkylation, with an olefin H2C:CR4CR5R6R7 (R4-R7 .noteq. H; do not interfere with a Friedel-Crafts-type alkylation) in presence of a Lewis acid and R8R9C:CR10CR11R12R13 (no more than 1 of R8-R10 = H; no more than 1 of R11-R13 = **H**) are **prepd.** in the absence of **iodine.** Cyclohexans and AlCl3 were cooled to 16.degree., and reacted with p-cymene, Me3CCH:CMe2 and Me3CCH:CH2 to give 1,2,3,4-tetrahydro-1,1,3,4,4,6-hexamethylnaphtahalene.
IT **107-40-4** **565-77-5**, 2,3,4-Trimethyl-2-pentene **598-96-9**, 3,4,4-Trimethyl-2-pentene **625-65-0**, 2,4-Dimethyl-2-pentene **126690-66-2**

(cycloaddn. of cymene with olefin in presence of)
RN 107-40-4 HCA
CN 2-Pentene, 2,4,4-trimethyl- (8CI, 9CI) (CA INDEX NAME)

```
Me2C== CH- Bu-t
```

RN 565-77-5 HCA
CN 2-Pentene, 2,3,4-trimethyl- (8CI, 9CI) (CA INDEX NAME)

```
    CMe2
    ||
Me- C- Pr-i
```

RN 598-96-9 HCA
CN 2-Pentene, 3,4,4-trimethyl- (8CI, 9CI) (CA INDEX NAME)

```
          Me
          |
Me- CH== C- Bu-t
```

RN 625-65-0 HCA
CN 2-Pentene, 2,4-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

```
Me2C== CH- Pr-i
```

RN 126690-66-2 HCA
CN 3-Heptene, 2,4,6-trimethyl- (9CI) (CA INDEX NAME)

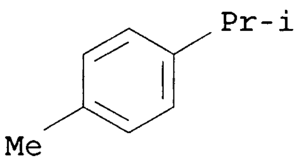
```
      Me
      |
i-Bu- C== CH- Pr-i
```

IT **558-37-2**, Neohexene
(cycloaddn. of, with cymene)
RN 558-37-2 HCA
CN 1-Butene, 3,3-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

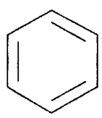
```
H2C== CH- Bu-t
```

IT **99-87-6**, p-Cymene **26573-16-0 29721-97-9**
126782-82-9
(cycloaddn. of, with olefins)

RN 99-87-6 HCA
CN Benzene, 1-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



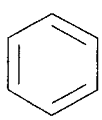
RN 26573-16-0 HCA
CN Benzene, ethyl(1-methylethyl)- (9CI) (CA INDEX NAME)



D1— Et

D1— Pr-i

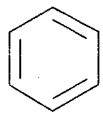
RN 29721-97-9 HCA
CN Benzene, (1,1-dimethylethyl)(1-methylethyl)- (9CI) (CA INDEX NAME)



D1— Pr-i

D1— Bu-t

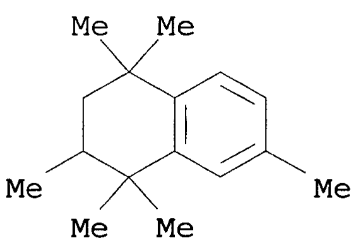
RN 126782-82-9 HCA
CN Benzene, (1-methylethyl)propyl- (9CI) (CA INDEX NAME)



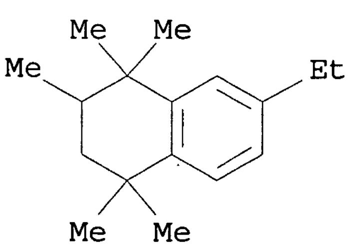
D1—Pr-i

D1—Pr-n

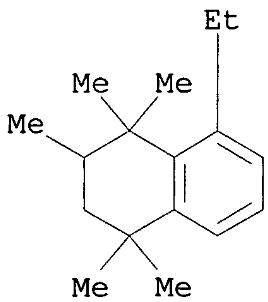
IT **2084-69-7P 5112-39-0P 126690-57-1P 126690-58-2P 126690-59-3P 126690-60-6P 126690-61-7P 126690-62-8P 126690-63-9P 126690-64-0P**
(prepn. of)
RN 2084-69-7 HCA
CN Naphthalene, 1,2,3,4-tetrahydro-1,1,2,4,4,7-hexamethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



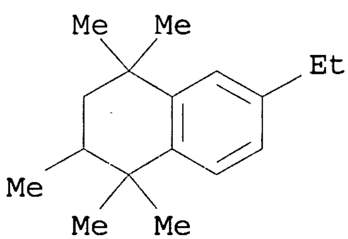
RN 5112-39-0 HCA
CN Naphthalene, 7-ethyl-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



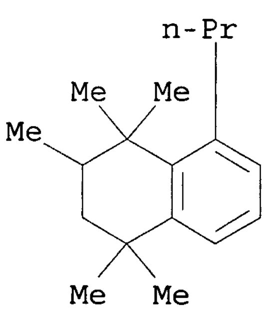
RN 126690-57-1 HCA
CN Naphthalene, 8-ethyl-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (9CI) (CA INDEX NAME)



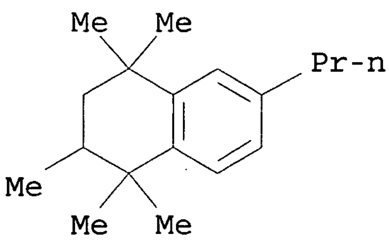
RN 126690-58-2 HCA
CN Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (9CI) (CA INDEX NAME)



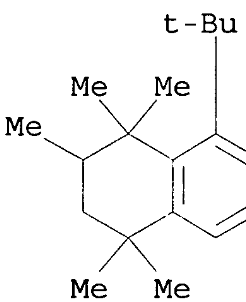
RN 126690-59-3 HCA
CN Naphthalene, 1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl-8-propyl- (9CI) (CA INDEX NAME)



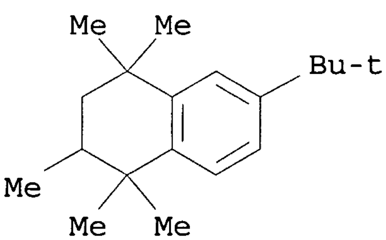
RN 126690-60-6 HCA
CN Naphthalene, 1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl-6-propyl- (9CI) (CA INDEX NAME)



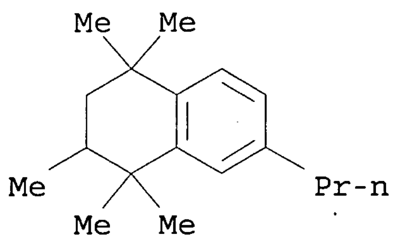
RN 126690-61-7 HCA
CN Naphthalene, 8-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (9CI) (CA INDEX NAME)



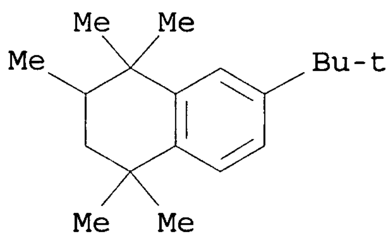
RN 126690-62-8 HCA
CN Naphthalene, 6-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (9CI) (CA INDEX NAME)



RN 126690-63-9 HCA
CN Naphthalene, 1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl-7-propyl- (9CI) (CA INDEX NAME)



RN 126690-64-0 HCA
CN Naphthalene, 7-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1,1,2,4,4-pentamethyl- (9CI) (CA INDEX NAME)



IC C07C012-00; C07C012-64; C07C002-64
INCL 585411000
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **107-40-4** **565-77-5**, 2,3,4-Trimethyl-2-pentene **598-96-9**, 3,4,4-Trimethyl-2-pentene **625-65-0**, 2,4-Dimethyl-2-pentene 5137-55-3, Methyltrioctylammonium chloride 7446-70-0, Aluminum chloride, reactions **126690-66-2**
(cycloaddn. of cymene with olefin in presence of)
IT **558-37-2**, Neohexene
(cycloaddn. of, with cymene)
IT **99-87-6**, p-Cymene **26573-16-0** **29721-97-9** **126782-82-9**
(cycloaddn. of, with olefins)
IT **2084-69-7P** **5112-39-0P** **126690-57-1P** **126690-58-2P** **126690-59-3P** **126690-60-6P** **126690-61-7P** **126690-62-8P** **126690-63-9P** **126690-64-0P**
(prepn. of)

L57 ANSWER 6 OF 32 HCA COPYRIGHT 2006 ACS on STN
100:121726 Electron-proton and electron-methyl exchanges in pyrolysis of polyacetylene and poly(methylacetylene). Chien, James C. W.; Fan, Ju Li (Dep. Chem., Univ. Massachusetts, Amherst, MA, 01003, USA). Pure and Applied Chemistry, 55(10), 1585-94 (English) **1983**. CODEN: PACHAS. ISSN: 0033-4545.

AB Pyrolysis of polyacetylene (I) [**25067-58-7**] gives high yields of **H**-rich **products**, e.g. CH_4, C_2H_4, C_2H_6, C_3H_8, C_3H_6, butadiene, cyclopentadiene, cyclopentene and PhMe, in total amts. exceeding that of **C_6H_6.** The activation energies for their formation are low. Conductive I doped with AsF_5 and **I_2** gave pyrolyzates in yields 2-17 times those of undoped I. The dominant mechanism is random chain scission followed by electron-H exchange. Poly(methylacetylene) (II) [**25684-85-9**] is less thermally stable than I, but also gives large amts. of proton enriched products with moderate activation energies. The yields of CH_4, C_2H_4, and C_2H_6 are nearly the same from I and II at 923 K; mechanisms of electron-H and -Me exchange are proposed to account for the products from II. These reactions, not obsd. in the pyrolysis of other polymers, result from the effect of the conjugated backbone on the facile migration of electrons, H, and Me groups.

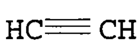
IT **25067-58-7 25684-85-9**
(pyrolysis of, mechanism of)

RN 25067-58-7 HCA

CN Ethyne, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-86-2
CMF C2 H2

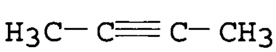


RN 25684-85-9 HCA

CN 2-Butyne, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 503-17-3
CMF C4 H6



CC 35-8 (Chemistry of Synthetic High Polymers)

IT **25067-58-7 25684-85-9**
(pyrolysis of, mechanism of)

L57 ANSWER 7 OF 32 HCA

98:16387 Acid-catalyzed intramolecular C-alkylation in .beta.,.gamma.-unsaturated diazomethyl ketones. 2. A simple new synthetic route to octahydro-4,10a-ethanophenanthren-12-ones and

octahydropentaleno[6a,1-a]naphthalen-4-ones. Satyanarayana, Gutta O. S. V.; Roy, Subhas C.; Ghatak, Usha Ranjan (Dep. Org. Chem., Indian Assoc. Cultiv. Sci., Calcutta, 700 032, India). Journal of Organic Chemistry, 47(27), 5353-61 (English) **1982.** CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 98:16387.

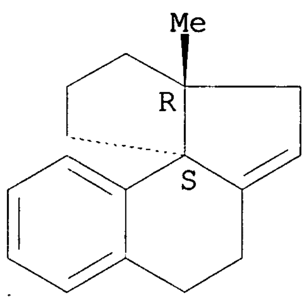
GI For diagram(s), see printed CA Issue.

AB The utility of acid-catalyzed intramol. C-alkylation and alkylation-rearrangements of the rigid diazomethyl ketones I (R1 = R2 = H; R1 = OMe, R2 = H; R1 = H, R2 = OMe) pertaining to a new and simple efficient synthesis of the resp. octahydro-4a-hydroxy-4,10a-ethanophenanthren-12-ones II and 3a-methylhexahydropentaleno[6a,1-a]naphthalen-4-ones III are described. The most thoroughly studied case was that of I (R1 = R2 = H) which clearly revealed that in a polar solvent, MeNO2, and with a strong protic acids or BF3.Et2O the hydroxycyclopentanone II (R1 = R2 = H) is the major product arising through the Wagner-Meerwein shifts of the initially generated resp. cyclobutanone carbinyl cation. While strong protic acids (aq. HClO4 or aq. HBF4) in nonpolar solvents (**C6H6** or CHCl3 contg. EtOH stabilizer) exclusively produce the unsatd. cyclobutanone IV (R1 = R2 = H), solvents of intermediate polarities with HBF4 or BF3.Et2O gave all 3 possible products, II, III, and IV (R1 = R2 = H). The structure of the products formed in the acid-catalyzed reactions of I (R1 = OMe, R2 = H; R1 = H, R2 = OMe) also depends upon the catalyst-solvent combinations as well as the reaction conditions and the nature of the substrates. The hydroxycyclopentanones II underwent facile rearrangement with 4-MeC6H4SO3H or **iodine** in refluxing **C6H6**, leading to the resp. pentaleno-annulated ketones III in excellent yields. These were also obtained from the resp. unsatd. cyclobutanones IV (R1 = OMe, R2 = H; R1 = H, R2 = OMe). The benzylic ketone V (R1 = R2 = **H**), **prepd.** in good yield through oxidn. of II (R1 = R2 = H), rearranged to the resp. enedione VI in excellent yield. Catalytic hydrogenolysis of the hydroxycyclopentanones II afforded the resp. bridged ketones VII exclusively. The stereochem. of VII (R1 = R2 = H; R1 = OMe, R2 = H) has been established by the x-ray method. The unsatd. cyclopentanones III undergo stereospecific hydrogenation to the resp. cis A-B cyclopentanones VIII whereas Li-liq. NH3 redn. of III (R1 = R2 = H, R1 = OMe, R2 = H) gives the resp. diastereoisomeric cyclopentanones VIII and IX in a ratio of .apprx.1:9 from which the major isomers were easily sepd. The ketone III (R1 = OMe, R2 = H) on the similar redn., however, gave an inseparable mixt. of VIII and IX (R's the same) of .apprx.1:2. The stereochems. of the epimeric ketones VIII and IX were assigned from the significant difference in the chem. shifts of the 3a-Me group in these diastereoisomeric pairs. The cyclopentenone III (R1 = R2 = H) has been transformed into the parent hydrocarbon X.

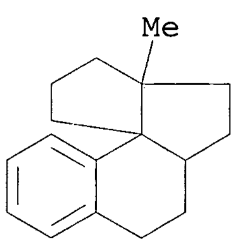
IT **83633-97-0P**

(prepn. and hydrogenation of)
RN 83633-97-0 HCA
CN 1H-Pentaleno[6a,1-a]naphthalene, 3,4,9,10,11,11a-hexahydro-11a-methyl-, (8bR*,11aS*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **83633-98-1P**
(prepn. of)
RN 83633-98-1 HCA
CN 1H-Pentaleno[6a,1-a]naphthalene, 2,2a,3,4,9,10,11,11a-octahydro-11a-methyl-, (2.alpha.,8bS*,11a.beta.)- (9CI) (CA INDEX NAME)



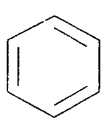
CC 25-28 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 83633-96-9P **83633-97-0P**
(prepn. and hydrogenation of)
IT 60103-66-4P 79958-94-4P 83633-90-3P 83633-91-4P 83633-92-5P 83633-93-6P 83633-94-7P **83633-98-1P** 83679-76-9P 83679-77-0P 83679-78-1P
(prepn. of)

L57 ANSWER 8 OF 32 HCA COPYRIGHT 2006 ACS on STN
95:71666 Intermolecular field interaction in solutions and effective dipole moment of **molecules. I.** Nonpolar solvents. Prezhdo, V. V.; Degtereva, L. I.; Lutskii, A. E. (Khar'k. Politekh. Inst., Kharkov, USSR). Zhurnal Obshchei Khimii, 51(4), 927-33 (Russian) **1981.** CODEN: ZOKHA4. ISSN: 0044-460X.
AB The effect of the intermol. field interaction on the effective

dipole moment of a mol. is estd. by using the London-Debye-Keesom potential for pair interactions of mols. in condensed media. Such an approach permits one to obtain a correlation of the elec. properties of mols. in solns. with characteristics of mol. structure of a liq. and thus to est. the contributions of different forms of field interaction in solns. Ref. data for the effective dipole moment in soln. were examd. in nonpolar solvents with similar ionization potential: heptane, hexane, **cyclohexane**, CCl4, dioxane, benzene, CS2, tetrachloroethylene, and **cyclohexane** . Dipole moments were measured of p-nitroanisole p-nitrodimethylaniline, o-nitrophenol, and salicylaldehyde in solns. Ar indicated dependence is satisfied by both compds. not **forming H** bonds and showing only field intermol. interactions. as well as compds. **forming** intermol. **H** bonds. For the presence in a mol. of dissolved material of several polar groups, the change of dipole moment is detd. not by local, but by the vol. character of the interaction with mols. of solvent.

IT **71-43-2**, properties **110-54-3**, properties
110-82-7, properties **110-83-8**, properties
142-82-5, properties
(effective dipole moment of mols. dissolved in)

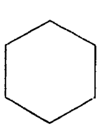
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



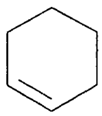
RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

Me—$(CH_2)_4$—Me

RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 110-83-8 HCA
CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



RN 142-82-5 HCA
CN Heptane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_5-Me$

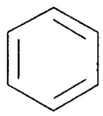
CC 76-3 (Electric Phenomena)
IT 56-23-5, properties **71-43-2**, properties 75-15-0, properties **110-54-3**, properties **110-82-7**, properties **110-83-8**, properties 123-91-1, properties 127-18-4, properties **142-82-5**, properties
(effective dipole moment of mols. dissolved in)

L57 ANSWER 9 OF 32 HCA COPYRIGHT 2006 ACS on STN
93:95873 Schiff base complexes. Riederer, Manfred (Fed. Rep. Ger.). Ger. Offen. DE 2834105 **19800221**, 33 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1978-2834105 19780803.
AB Polymeric Schiff base metal complexes were prepd. from diamines, bis(salicylaldehydes), and Group II-V metal ions, and contained channel-like voids, making them useful as chromatog. supports and adsorbents. Thus, 10 mmol 5,5'-methylenebissalicylaldehyde in 20 mL DMF was added to 4,4'-diaminodicyclohexylmethane 10, CrCl3.6H2O 11, and NaOAc 20 mmol in 100 mL DMF at 100.degree., heated 24 h at 100.degree., cooled, and filtered to give a yellow-green complex polymer (I) [69450-36-8]. I was used as a gas chromatog. stationary phase for sepg. a CO2-contg. mixt. which could not be sepd. on a zeolite because of partial irreversible absorption of the CO2. Relative retention times at 28.degree. and 30-40 mL/min were H 0.45, O 0.57, CO 0.65, N2O 0.758 CH4 0.98, and CO2 3.05 min. A Rh complex of one of the polymers was used as a hydrogenation catalyst.
IT **7553-56-2**, **Iodine**, properties
(adsorption of, from solns., Schiff base polymer metal complexes for)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

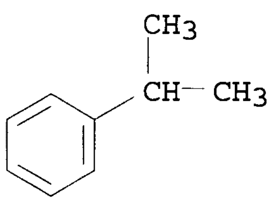
I—I

IT **71-43-2**, Benzene, properties
(adsorption of, on Schiff base polymer metal complexes)

RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



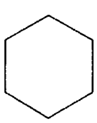
IT **98-82-8 109-66-0**, Pentane, properties
110-82-7, **Cyclohexane**, properties
1076-43-3, Benzene-d6
(adsorption of, on Schiff base polymer metal complexes)
RN 98-82-8 HCA
CN Benzene, (1-methylethyl)- (9CI) (CA INDEX NAME)



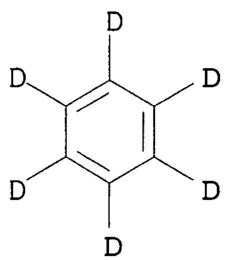
RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 1076-43-3 HCA
CN Benzene-d6 (8CI, 9CI) (CA INDEX NAME)



IT **74-82-8P**, Methane, **preparation**
(**hydrogen** sulfide removal from, adsorbents for)
RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

IT **592-41-6**, 1-Hexene, reactions
(hydrogenation of, catalyst for)
RN 592-41-6 HCA
CN 1-Hexene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}Bu\text{-}n$

IT **74-86-2**, Ethyne, uses and miscellaneous
(removal of, from air, Schiff base polymer metal complex adsorbents for)
RN 74-86-2 HCA
CN Ethyne (9CI) (CA INDEX NAME)

$HC{\equiv}CH$

IT **111-65-9**, Octane, uses and miscellaneous **540-84-1**
(sepn. of, by gas chromatog., stationary phases for)
RN 111-65-9 HCA
CN Octane (8CI, 9CI) (CA INDEX NAME)

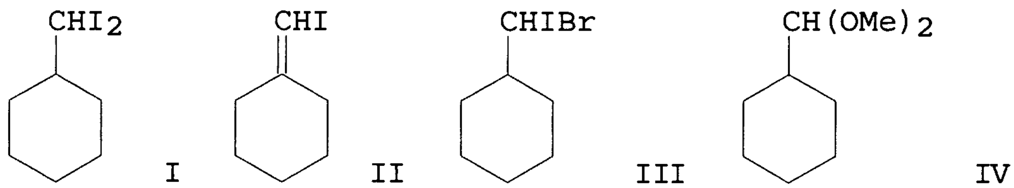
$Me{-}(CH_2)_6{-}Me$

RN 540-84-1 HCA
CN Pentane, 2,2,4-trimethyl- (8CI, 9CI) (CA INDEX NAME)

```
   Me
   |
Me—C—Bu-i
   |
   Me
```

IC C07D521-00
CC 35-3 (Synthetic High Polymers)
Section cross-reference(s): 78, 79
IT **7553-56-2**, **Iodine**, properties
(adsorption of, from solns., Schiff base polymer metal complexes for)
IT 56-23-5, properties 64-17-5, Ethanol, properties **71-43-2**
, Benzene, properties
(adsorption of, on Schiff base polymer metal complexes)
IT 79-01-6, properties **98-82-8** **109-66-0**, Pentane,
properties **110-82-7**, **Cyclohexane**, properties
110-86-1, Pyridine, properties **1076-43-3**, Benzene-d6
7732-18-5, Water, properties
(adsorption of, on Schiff base polymer metal complexes)
IT **74-82-8P**, Methane, **preparation**
(**hydrogen** sulfide removal from, adsorbents for)
IT **592-41-6**, 1-Hexene, reactions
(hydrogenation of, catalyst for)
IT **74-86-2**, Ethyne, uses and miscellaneous 74-90-8,
Hydrocyanic acid, uses and miscellaneous
(removal of, from air, Schiff base polymer metal complex adsorbents for)
IT **111-65-9**, Octane, uses and miscellaneous 124-38-9, Carbon
dioxide, uses and miscellaneous **540-84-1** 7439-90-9,
Krypton, uses and miscellaneous 7440-01-9, Neon, uses and
miscellaneous 7440-37-1, Argon, uses and miscellaneous
7440-59-7, Helium, uses and miscellaneous 7440-63-3, Xenon, uses
and miscellaneous 7727-37-9, Nitrogen, uses and miscellaneous
7782-44-7, Oxygen, uses and miscellaneous
(sepn. of, by gas chromatog., stationary phases for)

L57 ANSWER 10 OF 32 HCA COPYRIGHT 2006 ACS on STN
88:169310 Photochemistry of alkyl halides. 6. gem-Diiodides. A convenient method for the cyclopropanation of olefins. Pienta, Norbert J.; Kropp, Paul J. (Dep. Chem., Univ. North Carolina, Chapel Hill, NC, USA). Journal of the American Chemical Society, 100(2), 655-7 (English) **1978.** CODEN: JACSAT. ISSN: 0002-7863.
GI

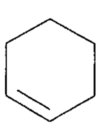


AB Irradn. of I in ether or **C6H6** afforded principally the vinyl iodide (II). In MeCN contg. LiBr or in MeOH the nucleophilic substitution products III or IV were obtained in addn. to II. In methylene chloride, 1,2-dichloroethane, and methylene bromide substantial quantities of 1-methylcyclohexene were obtained, which arose via acid-catalyzed isomerization of the primary product, methylenecyclohexane (V). Irradn. of I-1-d afforded V with substantial incorporation of D in the vinyl position, as expected from the formation of V via 1,2-insertion of a carbenoid intermediate. Irradn. of CH2I2 in CH2Cl2 soln. proved a convenient method for the high-yield cyclopropanation of cyclohexene, 2,3-dimethyl-2-butene, tert-butylethylene, and cis- and trans-3-hexene. The latter isomers underwent cyclopropanation with complete retention of stereochem. Cyclohexene and its 1-Me and 1,2-di-Me derivs. exhibited increasing reactivities with increasing degrees of substitution, in contrast with the Simmons-Smith procedure. In view of the lack of C-**H** insertion **products** the intermediacy of a methylene-**iodine** complex is proposed.

IT **110-83-8**, reactions **558-37-2** **563-79-1** **7642-09-3** **13269-52-8**
(photochem. cyclopropanation of, mechanism of)

RN 110-83-8 HCA

CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



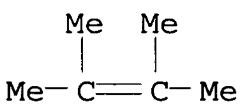
RN 558-37-2 HCA

CN 1-Butene, 3,3-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}Bu\text{-}t$

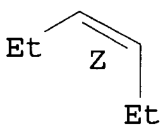
RN 563-79-1 HCA

CN 2-Butene, 2,3-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



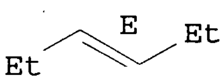
RN 7642-09-3 HCA
CN 3-Hexene, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

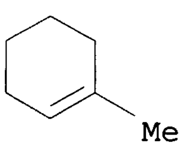


RN 13269-52-8 HCA
CN 3-Hexene, (3E)- (9CI) (CA INDEX NAME)

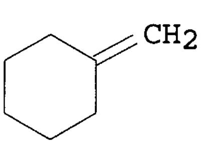
Double bond geometry as shown.



IT **591-49-1P 1192-37-6P**
(prepn. of)
RN 591-49-1 HCA
CN Cyclohexene, 1-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 1192-37-6 HCA
CN Cyclohexane, methylene- (8CI, 9CI) (CA INDEX NAME)



CC 22-4 (Physical Organic Chemistry)
IT **110-83-8**, reactions **558-37-2 563-79-1**
7642-09-3 13269-52-8

(photochem. cyclopropanation of, mechanism of)
IT **591-49-1P** **1192-37-6P** 18231-08-8P 23904-33-8P
65826-86-0P
(prepn. of)

L57 ANSWER 11 OF 32 HCA COPYRIGHT 2006 ACS on STN
78:96842 Synthesis of methylacetylene by the pyrolysis of propylene. VII. Catalysis by **iodine.** Taniuchi, Mamoru (Inst. Chem. Res., Kyoto Univ., Kyoto, Japan). Bulletin of the Institute for Chemical Research, Kyoto University, 50(4), 383-92 (English) **1972.** CODEN: BICRAS. ISSN: 0023-6071.
AB Propene was pyrolyzed with **iodine** catalyst and N diln. over a wide range of conditions. The main **products** were **H**, CH4, CH.tplbond.CH, CH2:CH2, CH2:C:CH2 (I), MeC.tplbond.CH (II), Ch2:CHCH:CH2, **C6H6**, and Me2CHI. Optimum conditions were detd. for the formation of I and II. Radical mechanisms were discussed.
IT **7553-56-2**, uses and miscellaneous
(catalysts, for pyrolysis of propene to allene and propyne)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

$I-I$

IT **74-99-7P** **463-49-0P**
(prepn. of)
RN 74-99-7 HCA
CN 1-Propyne (9CI) (CA INDEX NAME)

$H_3C-C\equiv CH$

RN 463-49-0 HCA
CN 1,2-Propadiene (9CI) (CA INDEX NAME)

$H_2C=C=CH_2$

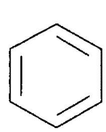
IT **115-07-1**, reactions
(pyrolysis of, allene and propyne by)
RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

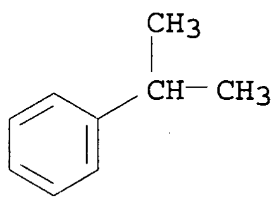
CC 22-4 (Physical Organic Chemistry)

IT **7553-56-2**, uses and miscellaneous
(catalysts, for pyrolysis of propene to allene and propyne)
IT **74-99-7P 463-49-0P**
(prepn. of)
IT **115-07-1**, reactions
(pyrolysis of, allene and propyne by)

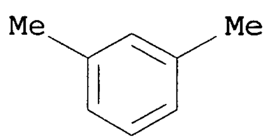
L57 ANSWER 12 OF 32 HCA COPYRIGHT 2006 ACS on STN
77:80036 Distribution of diaminodiphenylmethane isomers between organic solvents and water. Korenman, I. I.; Gur'ev, I. A.; Tsigin, B. M. (USSR). Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin., No. 1, 57-64 From: Ref. Zh., Khim. 1971, Abstr. No. 15B724 (Russian) **1971.**
AB A photocolorimetric method was used at 20 .+-. 1.degree. to study the distribution of 4,4'-, 4,2'-, 3,3'-, and 2,2'-(H2NC6H4)2CH2 (I), which are basic components of polyamine, between aq. soln. (pH 10, [I] = 10-4-3.8 .times. 10-3M) and org. solvents C7H16, C15H32, **C6H12**, CCl4, C2Cl4, **C6H6**, PhMe, m-Me2C6H4, iso-PrPh, PhCl, o-Cl2C6H4, 1,2,4-C6H3Cl3, PhBr, PhI, CHCl3, CH2Cl2, C2H4Cl2, CHBr3, C2HCL3, PhNO2, EtOAc, n-C5H11OAc, PhCH2OAc, PhOMe, iso-Pr2O, n-C6H13OH, sec-C6H13OH, tert-C6H13OH, n-C7H15OH, C8H17OH, and PhCH2OH. The aq. and the org. phases were mutually satd. prior to extn. Mixing time was 10 min. The distribution coeffs. (P) of I were tabulated as a function of [I]. The I in both phases exist as nonassocd. mols. and the P are thermodynamic consts. Min. P were obsd. for the solns. where the **formation** of **H** bonds is not characteristic. The P for aliphatic solvents is somewhat less than for aromatic solvents. The P increased with transfer of the amino group in I from the para position to meta and ortho-positions. The P for **C6H6** and its homologs decreased with increase of the mol. vol. of a solvent. The log P for halo-substituted **C6H6** increased with decrease of the electronegativity of substituents in the Cl-Br-**iodine** order. The log P increased linearly with increase of the water soly. log in the solvents in question.
IT **71-43-2**, properties **98-82-8 108-38-3**, properties **108-88-3**, properties **110-82-7**, properties **142-82-5**, properties **629-62-9**
(partition of diaminodiphenylmethane isomers between aq. soln. and)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



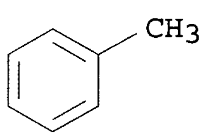
RN 98-82-8 HCA
CN Benzene, (1-methylethyl)- (9CI) (CA INDEX NAME)



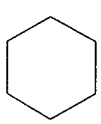
RN 108-38-3 HCA
CN Benzene, 1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 142-82-5 HCA
CN Heptane (8CI, 9CI) (CA INDEX NAME)

Me— $(CH_2)_5$—Me

RN 629-62-9 HCA
CN Pentadecane (6CI, 8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_{13}-Me$

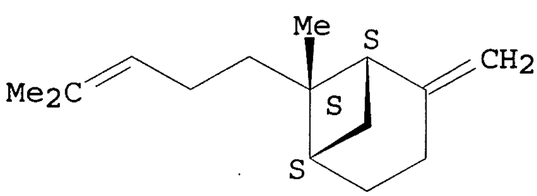
CC 68-1 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
IT 56-23-5, properties 67-66-3, properties **71-43-2**, properties 75-09-2 75-25-2 79-01-6 95-50-1 **98-82-8** 98-95-3, properties 100-51-6 100-66-3 108-20-3 **108-38-3**, properties 108-86-1 **108-88-3**, properties 108-90-7, properties **110-82-7**, properties 111-27-3 111-70-6 111-87-5 120-82-1 127-18-4 140-11-4 141-78-6, properties **142-82-5**, properties 591-50-4 628-63-7 **629-62-9** 1300-21-6 26401-20-7 37769-60-1
(partition of diaminodiphenylmethane isomers between aq. soln. and)

L57 ANSWER 13 OF 32 HCA
67:11603 Stereospecific synthesis of cis-.beta.-bergamotene. Gibson, Thomas W.; Erman, William F. (Procter and Gamble Co., Cincinnati, OH, USA). Tetrahedron Letters (10), 905-9 (English) **1967.** CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 67:11603.
GI For diagram(s), see printed CA Issue.
AB Ozonolysis of (-)-.beta.-pinene followed by addn. of MeLi gave the alc. (I, R = Me) (II). II treated with Pb(OAc)4 and **iodine** in **cyclohexane** under irradn. from a tungsten lamp yielded 80-92% cyclic ether (III, R = Me) (IV). Similar results could be obtained under more convenient conditions by treatment of II with HgO and Br in refluxing pentane. IV b10.5 64.degree., n26D 1.4702, [.alpha.]5461 51.7.degree. (c 3.0, alc.). Similar treatment of alcs. I (R = **H**, CH2CO2Et), **prepd.** by LiAlH4 redn. and the Reformatskii reaction, resp., with nopinone, gave nearly quant. yields of the cyclic ethers III (R = H, CH2CO2Et). Mild hydrolysis of the etherester gave the corresponding carboxylic acid, converted by treatment with Pb(OAc)4 and NaCl in refluxing CCl4 to 54% .beta.-chloro ether (V), b1.3 65.degree.. Treatment of V in refluxing monoglyme with Na yielded 48% alc. (VI, R = H) (VII), b0.5 55.degree., converted by acids and by chromatog. to IV. IV was converted under mild conditions to the cryst. tosylate VI (R = SO2C6H4Me-p), and transformed by treatment with NaI in refluxing Me2CO to the iodide (VIII). Formation of the Grignard reagent of VIII followed by quenching with H2O gave only the monocyclic dienes, limonene and p-mentha-1(7),8-diene, thus preventing the use of a coupling reaction for the synthesis of the desired hydrocarbon. Treatment of VIII with the LiC.tplbond.CH.H2NCH2CH2NH2 complex in Me2SO yielded 71% acetylenic olefin (IX), [.alpha.]5461 41.degree. (c 1.95, alc.), hydroborated with (Me2CHCH2CH2)2BH2 and the product oxidized to give the unstable aldehyde (X), b0.6 95.degree.. Treatment of X with Me2C:PPH3 in tetrahydrofuran yielded 32% (from IX) hydrocarbon (XI), b0.5 105-25.degree., [.alpha.]25D 40.2.degree.

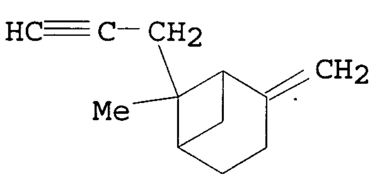
(c 1.74, CHCl3). In .beta.-bergamotene (XII), the signal for the Me group on the quaternary C atom appears at 8.78 suggesting the assigned structure. The N.M.R. and ir spectra of the above compds. are reported.

IT **15438-93-4**
(as structure for cis-.beta.-bergamotene)
RN 15438-93-4 HCA
CN Bicyclo[3.1.1]heptane, 6-methyl-2-methylene-6-(4-methyl-3-pentenyl)-, (1S,5S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

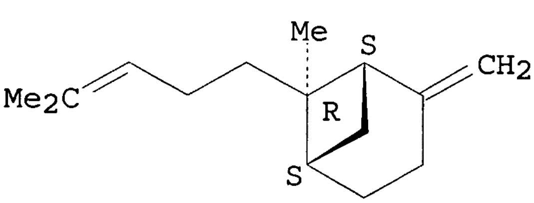


IT **15371-30-9P 15438-94-5P**
(prepn. of)
RN 15371-30-9 HCA
CN Norpinane, 6-methyl-2-methylene-6-(2-propynyl)-, (1S,5S,6S)-(+)-(8CI) (CA INDEX NAME)



RN 15438-94-5 HCA
CN Bicyclo[3.1.1]heptane, 6-methyl-2-methylene-6-(4-methyl-3-pentenyl)-, (1S,5S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



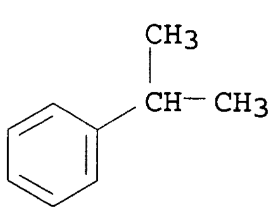
CC 30 (Terpenes)

IT **15438-93-4**
(as structure for cis-.beta.-bergamotene)
IT 7663-67-4P 15371-24-1P 15371-25-2P 15371-26-3P 15371-27-4P
15371-28-5P 15371-29-6P **15371-30-9P** **15438-94-5P**
15448-07-4P
(prepn. of)

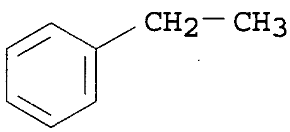
L57 ANSWER 14 OF 32 HCA COPYRIGHT 2006 ACS on STN
65:20423 Original Reference No. 65:3755b-d Improved method of oxidative dehydrogenation. Blood, A. E.; Hagemeyer, H. J., Jr. (Eastman Kodak Co.). BE 667996 **19660207**, 26 pp. (Unavailable).
PRIORITY: US 19640807.

AB Improvements to the known method of oxidative dehydrogenation of satd. org. compds., catalyzed by **iodine** compds., with higher yields and low loss of **iodine**, are cited. The catalyst used is HI hydrate, added at a rate of 0.5-10.0 wt. % to the compd. to be dehydrogenated. O is present in a 1:3-1:10 mole ratio to the org. compd., and the reaction run >400.degree.. The product is cooled by water or mother liquors, and the ethylenic compd. is sepd. from **iodine.** The satd. org. compd. used must contain at least two vicinal aliphatic hydrogenated C atoms, or a C>2 alkyl group, preferably Et or iso-Pr. A design of corrosion-resistant equipment is given with a detailed description of the oxidative dehydrogenation of Me2CHCO2Me (I) to CH2: CMeCO2Me (II). Thus, I in aq. HI (100:2 by wt. I-HI) was preheated to 450.degree., mixed with air (I-O mole ratio 10:2), the mixt. passed through a Vycor tube filled with Vycor chips and heated at 600.degree. at a rate of 600 cc. per cc. reactor per hr., the tube effluent absorbed in water, and the liquid product sepd. to give 72% II (13% conversion). No CH2:CHCO2Me was formed, and the raw product contained only a trace of catalyst and no **iodine**; 95% catalyst was recovered for recycle. Similarly prepd. were (% conversion and % yield given): styrene 23, 78; .alpha.-methyl-styrene 35, 85.5; **C6H6** (from **cyclohexane**) 45, 94; CH2:CMe2 25, 94; MeCH2CH: CMeCO2Me, 26, --; methyl 2-ethylhexeno-ates, 24, --; CH2:CMeCO2H, 18.5, --.

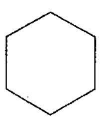
IT **98-82-8**, Cumene **100-41-4**, Benzene, ethyl-
(dehydrogenation of)
RN 98-82-8 HCA
CN Benzene, (1-methylethyl)- (9CI) (CA INDEX NAME)



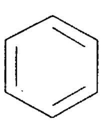
RN 100-41-4 HCA
CN Benzene, ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



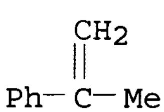
IT **110-82-7**, **Cyclohexane**
(dehydrogenation of, oxidative)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



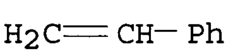
IT **71-43-2**, Benzene **98-83-9**, Styrene, .alpha.-methyl-
100-42-5, Styrene **115-11-7**, Propene, 2-methyl-
(isobutylene)
(manuf. of)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



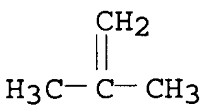
RN 98-83-9 HCA
CN Benzene, (1-methylethenyl)- (9CI) (CA INDEX NAME)



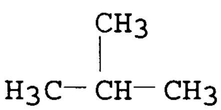
RN 100-42-5 HCA
CN Benzene, ethenyl- (9CI) (CA INDEX NAME)



RN 115-11-7 HCA
CN 1-Propene, 2-methyl- (9CI) (CA INDEX NAME)



IT **75-28-5**, Propane, 2-methyl-
(oxidative dehydrogenation of)
RN 75-28-5 HCA
CN Propane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



CC 33 (Aliphatic Compounds)
IT **98-82-8**, Cumene **100-41-4**, Benzene, ethyl-
(dehydrogenation of)
IT **110-82-7**, **Cyclohexane**
(dehydrogenation of, oxidative)
IT **71-43-2**, Benzene 80-62-6, Methyl methacrylate
98-83-9, Styrene, .alpha.-methyl- **100-42-5**,
Styrene **115-11-7**, Propene, 2-methyl- (isobutylene)
10478-12-3, 2-Pentenoic acid, 2-methyl-, methyl ester
(manuf. of)
IT **75-28-5**, Propane, 2-methyl- 79-31-2, Isobutyric acid
107-12-0, Propionitrile 554-12-1, Propionic acid, methyl ester
816-19-3, Hexanoic acid, 2-ethyl-, methyl ester 2177-77-7, Valeric
acid, 2-methyl-, methyl ester
(oxidative dehydrogenation of)
IT 123-94-4, Stearin, 1-mono- 6170-45-2, Glycerol, 1-salicylate
10482-23-2, Glycerol, 1,1'-bis(**hydrogen** adipate)
875823-81-7, Glycerol, 1,1',1''-tris(di-**H** citrate)
(**prepn.** of)

L57 ANSWER 15 OF 32 HCA COPYRIGHT 2006 ACS on STN
64:103973 Original Reference No. 64:19520a-h,19521a-c
Spiro-di-.omicron.-xylylene. Errede, Louis A. (Minnesota Mining and
Manufacturing Co.). US 3242205 **19660322**, 6 pp.
(Unavailable). APPLICATION: US 19591202. PRIORITY: US 19591202.

L57 ANSWER 16 OF 32 HCA COPYRIGHT 2006 ACS on STN
63:97474 Original Reference No. 63:17838e-h Recoil chemistry of
carbon-11 in liquid hydrocarbons. Clark, Donald Eldon (Iowa State
Univ. of Sci. & Technol., Ames). U.S. At. Energy Comm., IS-T-23, 93

pp. (English) **1965.**

AB The chem. behavior of recoil carbon-11 atoms in various C5-7 hydrocarbons has been investigated. The recoil atoms were produced by the 12C(.gamma.,n)11C reaction with the bremsstrahlung beam of an electron synchrotron. Standard gas chromatographic methods coupled with scintillation flow counting techniques were used for radioassay of the labeled products. This study was principally concerned with the product yields of ethane, ethylene, and acetylene from the different target compounds, although methane yields were also detd. in all cases. The initial phase of the investigation established the effects of **iodine** as a radical scavenger and radiation dose on the product yields. **Iodine** affected the yields of all of the volatile products except acetylene. Radiation dose had the effect of changing the yields; the changes appeared to be primarily due to radiolytically **produced hydrogen** which was able to reduce some of the labeled species. When irradiation times of about five min. or less were used, the results were approx. the same as would have been obtained for the idealized zero dose case. The two-carbon product yields, as well as the (C2H6 + C2H4/C2 ratios, were shown to be dependent upon the structure of the target mols. These results are discussed in terms of the decompn. modes available to the assumed activated complexes resulting from insertion-type reactions of three primary species 11C, 11CH and 11CH2. Mixts. of benzene and methylcyclopentane were irradiated and the yields of volatile products were detd. Within exptl. error, the yields were shown to be strictly dependent upon the molar concns. of the two components. This was interpreted as being an indication that the reaction cross sections for equiv. labeled species with the two different mols. have similar energy dependences. This study appears to confirm that 3 neutral species, 11C, 11CH and 11CH2, are responsible for the products formed in these systems. The reactions by which the products are formed seem to proceed via mechanisms involving the insertion of these three recoil fragments into C-H and C:C bonds of the parent compds.

IT **109-66-0**, Pentane **110-54-3**, Hexane
110-82-7, Cyclohexane
(carbon-11 hot-atom chemistry in .gamma.-irradiated)

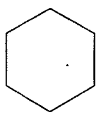
RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C—CH_2—CH_2—CH_2—CH_3$

RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me—(CH_2)_4—Me$

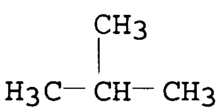
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



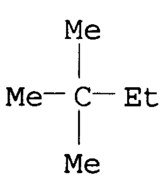
IT **74-98-6**, Propane **75-28-5**, Propane, 2-methyl-
75-83-2, Butane, 2,2-dimethyl- **79-29-8**, Butane,
2,3-dimethyl- **96-14-0**, Pentane, 3-methyl- **107-83-5**
, Pentane, 2-methyl- **108-87-2**, **Cyclohexane**,
methyl- **108-88-3**, Toluene **592-41-6**, 1-Hexene
592-43-8, 2-Hexene
(carbon-11 hot-atom reactions in .gamma.-irradiated)
RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

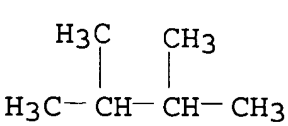
RN 75-28-5 HCA
CN Propane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 75-83-2 HCA
CN Butane, 2,2-dimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 79-29-8 HCA
CN Butane, 2,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



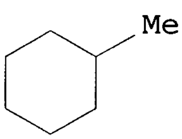
RN 96-14-0 HCA
CN Pentane, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

```
    Me
    |
Et— CH— Et
```

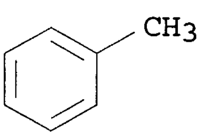
RN 107-83-5 HCA
CN Pentane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)

```
    Me
    |
Me— CH— Pr-n
```

RN 108-87-2 HCA
CN Cyclohexane, methyl- (8CI, 9CI) (CA INDEX NAME)



RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



RN 592-41-6 HCA
CN 1-Hexene (8CI, 9CI) (CA INDEX NAME)

H_2C═CH— Bu-n

RN 592-43-8 HCA
CN 2-Hexene (8CI, 9CI) (CA INDEX NAME)

n-Pr— CH═CH— Me

IT **7553-56-2, Iodine**

(carbon-11 hot-atom reactions in .gamma.-irradiated liquid hydrocarbons in presence of)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

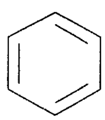
I—I

IT **71-43-2**, Benzene

(carbon-11 hot-atom reactions in .gamma.-irradiated, methylcyclopentane and)

RN 71-43-2 HCA

CN Benzene (8CI, 9CI) (CA INDEX NAME)

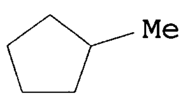


IT **96-37-7**, Cyclopentane, methyl-

(11C hot-atom reactions in .gamma.-irradiated)

RN 96-37-7 HCA

CN Cyclopentane, methyl- (8CI, 9CI) (CA INDEX NAME)



CC 32 (Physical Organic Chemistry)

IT **109-66-0**, Pentane **110-54-3**, Hexane **110-82-7**, **Cyclohexane**

(carbon-11 hot-atom chemistry in .gamma.-irradiated)

IT **74-98-6**, Propane **75-28-5**, Propane, 2-methyl- **75-83-2**, Butane, 2,2-dimethyl- **79-29-8**, Butane, 2,3-dimethyl- **96-14-0**, Pentane, 3-methyl- **107-83-5**, Pentane, 2-methyl- **108-87-2**, **Cyclohexane**, methyl- **108-88-3**, Toluene **592-41-6**, 1-Hexene **592-43-8**, 2-Hexene

(carbon-11 hot-atom reactions in .gamma.-irradiated)

IT **7553-56-2**, **Iodine**

(carbon-11 hot-atom reactions in .gamma.-irradiated liquid hydrocarbons in presence of)

IT **71-43-2**, Benzene

(carbon-11 hot-atom reactions in .gamma.-irradiated, methylcyclopentane and)

IT **96-37-7**, Cyclopentane, methyl-

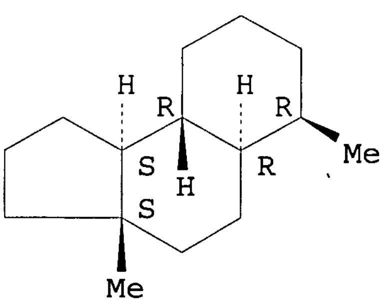
(11C hot-atom reactions in .gamma.-irradiated)

L57 ANSWER 17 OF 32 HCA COPYRIGHT 2006 ACS on STN
60:30580 Original Reference No. 60:5353e-h,5354a-d Synthesis and polymerization of 3-azabicyclo[4.3.1]decan-4- one and 7,7-dimethyl-2-azabicyclo[4.1.1]octan-3-one. Hall, H. K. Jr. (E. I. du Pont de Nemours, Wilmington, DE). Journal of Organic Chemistry, 28(11), 3213-14 (Unavailable) **1963.** CODEN: JOCEAH. ISSN: 0022-3263.
GI For diagram(s), see printed CA Issue.
AB cf. CA 54, 17292e. EtOH (520 ml.) and 2.5 l. **C6H6** contg. 315 g. 1: 1 m- and p-HO2CCH2C6H4CH2CO2H (I) refluxed 1 hr. with stirring and the chilled mixt. filtered gave 117 g. almost **pure I**, m. 255.degree.. The filtered soln. concd., dild. with 1.2 l. EtOH, satd. with dry HCl 20 hrs., and distd. gave 217 g. di-Et phenylenediacetates, b1.1 127-30.degree., hydrogenated in 250 ml. alc. at 135.degree. and 1565 lb./in.2 over 3 g. RuO2 with adsorption of 1.4 moles **H**, the **product** (174.5 g., b0.15 115-33.degree.) refluxed (70.0 g.) 5 hrs. with 70 g. NaOH in 500 ml. 2:3 alc.-H2O, the alc. evapd., the residue cooled, acidified with 12N HCl, and kept 3 days, and the ppt. rinsed with H2O gave 51.0 g. air-dried 1,3- and 1,4-cyclohexanediacetic acids, m. 130-2.degree.. The acid mixt. (26.0 g.) and 50 ml. Ac2O distd. 1 hr. with passage of AcOH, the remainder distd. through a Claisen head at 150 mm., the distillate taken up in 100 ml. Et2O and washed with 100 ml. H2O and 150 ml. 15% aq. Na2CO3, the aq. layers extd. with 50 ml. C6H14, the dry org. layers evapd., the residue submitted to short path distn. at 15 mm., the residue crystd. at -80.degree. from C6H14, and the solid (4.6 g.) sublimed at 140.degree./18 mm. yielded 22.6% pure bicyclo[3.3.1]nonan-3-one (II), m. 180-2deg;, .lambda. 1706, 1717 cm.-1; 2,4- dinitrophenylhydrazone m. 208-9.degree. (alc.-EtOAc). Use of BaO in place of Ac2O in the distn. gave a lower yield of II. Esterification of I and hydrogenation of the di-Et ester, m. 59.0-9.5.degree. gave di-Et **cyclohexane**-1,4-diacetate, hydrolyzed to **cyclohexane**-1,4-diacetic acid, m. 164-5.degree. and distd. from-BaO without production of ketonic material showed that II was derived from **cyclohexane** -1,3-diacetic acid. II (12.79 g.) was converted with HONH2 (loc. cit.) to a white solid, m. 108-14.degree., in the receiver to give a crude oxime (12.25 g., b1.0 113-15.degree.), which recrystd. from 30 ml. **C6H6** yielded 71.3% oxime (III), m. 108-9.degree.. III (9.92 g.) submitted to Beckmann rearrangement with PhSO2Cl (Gates and Malchick, CA 52, 4507b) gave 6.2 g. lactam, subliming at 100-60.degree./0.45 mm., recrystd. from 25 ml. C6H14 at -80.degree. yielded 55.9% 3-azabicyclo[4.3.1]decan-4-one (IV). Similar cyclization of **cyclohexane**-1,4-diacetic acid gave no bicyclo[3.2.2]nonan-3-one (V). The ketone II can exist in a stable

two-chair conformation, whereas V would have a strained boat form of the **cyclohexane** ring, thus accounting for the difference in ease of formation of the 2 ketones. Com. .beta.-pinene (91% pure "sulfate" pinene, Hercules Powder Co.) ozonized according to Meinwald and Gassman (CA 55, 7314e) gave 99% pure nopinone, b16 92.degree., converted (38.2 g.) to the oxime and distd. to give 40.1 g. material, b1.5 107.degree., recrystd. from 20 ml. C7H16, to yield 33.2 g. nopinone oxime (VI), m. 61.5-5.0.degree.. VI (23.1 g.) submitted to the Beckman rearrangement by using NaOH and PhSO2Cl], the CHCl3 ext. concd. and dild. with 800 ml. Et2O, the filtered soln. concd. and distd. at 0.3 mm. up to 130.degree., and the solidified distillate sublimed 3 times and crystal. from 15 ml. C7H16 yielded 42.6% 7,7-dimethyl-2-azabicyclo[4.1.1]octan-3-one (VII), m. 111-13.degree., showing an infrared spectrum consistent with that of a lactam but no observable 6.50 .mu. band. IV (1.50 g.) heated with a drop of H2O and a drop of 85% H3PO4 8.5 hrs. at 223.degree. in a sealed glass tube under N and the product washed with H2O and Me2CO yielded 88% polyamide of cis-3-aminomethylcyclo-hexylacetic acid, m. 297.degree., inherent viscosity 0.21, in m-cresol. Similar polymerization of VII with 5% 85%. H3PO4 at 200.degree. in 17 hrs. followed by extn. with MeOH yielded 75% polyamide of cis-3-amino-2,2-dimethylcyclobutanepropionic acid, m. 358.degree., inherent viscosity 0.62 in m-cresol. Use of less H3PO4 for longer periods gave lower mol. wt. polymer, and the use of NaH-Ac2O produced only dark oils.

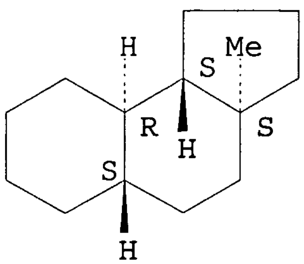
IT **782478-34-6**, De-A-androstane
(derivs)
RN 782478-34-6 HCA
CN De-A-androstane (7CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **66375-71-1**, De-A-estrane
(derivs.)
RN 66375-71-1 HCA
CN 1H-Benz[e]indene, dodecahydro-3a-methyl-, [3aS-(3a.alpha.,5a.beta.,9a.alpha.,9b.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

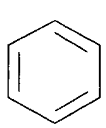


CC 34 (Alicyclic Compounds)
IT **782478-34-6**, De-A-androstane
(derivs)
IT **66375-71-1**, De-A-estrane
(derivs.)

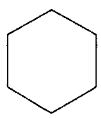
L57 ANSWER 18 OF 32 HCA COPYRIGHT 2006 ACS on STN
59:41327 Original Reference No. 59:7399a-h Hexafluoro- and perchlorofluorobenzenes from perchlorofluorocyclohexanes and cyclohexenes. Chambers, R. D.; Heyes, J.; Musgrave, W. K. R. (Univ. Durham, UK). Tetrahedron, 19(6), 891-900 (Unavailable) **1963**. CODEN: TETRAB. ISSN: 0040-4020.
GI For diagram(s), see printed CA Issue.
AB cf. CA 58, 462c. ClF3 (55 g.) dild. with N (5 l./hr. 1st hr., then 2.5 l./hr.) passed at 240.degree. into 100 g. molten C6Cl6 at 20-5 g./hr. 1st hr. and 10-15 g./hr. thereafter, with vigorous stirring and a wide air condenser, the mixt. swept 30 min. with N and dild. with Et2O, filtered and the washed (N NaOH, H2O) and dried filtrate evapd., the product distd. through a 20-plate concentric-tube column and each fraction purified by preparative scale gas-chromatography using silicone elastomer as the stationary phase gave the following chlorofluorocyclohexenes (% compn. based on 90% **C6H6**) [component, % yield, b.p., and nD/temp, given]: C6F5Cl5 (I), 2, 148.degree., 1.4050/20.degree., 1.4006/30.degree.; C6F6Cl4 (II), 10, 178.5.degree., 1.4367/20.degree.; C6F4Cl4 (III), 4, - (m.p. 46.5.degree.), -; C6F5Cl5, 30, 208.5.degree., 1.4699/20.degree.; C6F4Cl6, 35, 242.5.degree., 1.4998/20.degree.; C6Cl6, 10, - (m. 227.degree.), -. C6F8Cl2 (IV) and I, prepd. commercially by the action of SbF3 on C6Cl6, were purified by preparative gas-chromatography. The spectral data proved that III had the structure shown. CIF3 (55 g.) added as above to 100 g. C6Cl6, the temp. lowered to 100.degree., and 184 g. ClF3 dild. with N (2.5 l./hr.) added in 18 hrs., the following chlorofluorocyclohexanes isolated, and the identities established (except for C6F6Cl6 and C6F7Cl5) by comparison, using gas-chromatography, with the

corresponding compd. prepd. from C6Cl6 and Co2F6 (compd., % yield, b.p., and m.p. given): C6F9Cl3, trace, 142.degree., -;C6F8Cl4, 10, 175.5.degree., -; C6F7Cl5, 25, 207.5.degree. 74-6.degree.; C6F8Cl8, 15, 248.degree., 103-5.degree.; C6F5Cl7, 2, 270-3.degree., 105-10.degree.. A few expts. using only 100% excess ClF3 in the presence of catalysts showed that CoF2 encouraged satn. but also promoted decompn., whereas FeCl2 increased the proportion of the more highly fluorinated product with increased decompn., and BF2 gave results little better than those obtained in the absence of catalyst. The chlorofluorocyclohexenes and III were flash-distd. at 5 g. in 20 min. in a stream of N (60 ml./min.) over a tightly packed roll of Fe gauze in a mild steel tube (44 in. .times. 2 in.) heated by electrical strip heaters to maintain a const. temp. in the central 20-in. portion. The products were collected in liquid air-cooled traps and sepd. by preparative scale gas-chromatography. The % compn. of the roomers of the chlorofluorobenzenes were detd. by nuclear magnetic resonance spectroscopy. The 1st sample of each compd. was identified by Cl and F analysis and by infrared spectroscopy (compd., b.p., n20D, m.p., and mol. wt. given): C6F6, 79.0.degree., 1.3765, -, -; C6F5Cl, 117.5.degree., 1.4188, -, 206; C6F4Cl2, 150.5.degree., 1.4659, -, 230; C6F8Cl3, 23.5.degree., 245; C6F2CI4, 62.degree., -; C6FCl5, -, -,134.degree.,-. Dehalogenation of chlorofluorocyclohexanes were carried out under similar conditions at 260-430.degree.. Liquid phase halogenation of C5Cl6 appears to proceed by a series of addns. and vinylic and allylic substitutions until C6Cl6 is converted into chlorofluorocyclohexenes, C6Fn Cl12 n (where n is mainly 4, 5, and 6). A very large excess of ClF3 gives chlorofluorocyclohexanes, C6FnCl12-n (where n is mainly 5, 6, and 7). Aromatization of cyclohexenes at 200-300.degree. gives all possible chlorofluorobenzenes whereas that of cyclo-hexanes at 250-300.degree. gives mainly C6F6Cl and C6F4Cl2, with some C6F6 and C6F3Cl3. At the low temps. used there is little opportunity for rearrangement within the mol. and this results in the retention of Cl atoms in the aromatic products. The distribution of isomers of the aromatic products sheds some light on the structures of the chlorofluorocyclohexenes and -**cyclohexanes** from which they are.derived, and hence on the mechanism of halogenation.

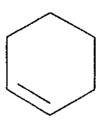
IT **71-43-2**, Benzene
(derivatives, halo)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



IT **110-82-7**, **Cyclohexane** **110-83-8**,
Cyclohexene
(halo derivs.)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



RN 110-83-8 HCA
CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



CC 35 (Noncondensed Aromatic Compounds)
IT Halogens
(removal of, from chloro fluoro **cyclohexane** derivs.)
IT **71-43-2**, Benzene
(derivatives, halo)
IT **110-82-7**, **Cyclohexane** **110-83-8**,
Cyclohexene
(halo derivs.)
IT 319-87-9, Benzene, pentachlorofluoro- 319-88-0, Benzene,
1,3,5-trichloro-2,4,6-trifluoro- 336-19-6, Cyclohexene,
1,2-dichlorooctafluoro- 344-07-0, Benzene, chloropentafluoro-
392-56-3, Benzene, hexafluoro- 827-12-3, Benzene,
1,2,3-trichloro-4,5,6-trifluoro- 827-13-4, Benzene,
1,2,4-trichloro-3,5,6-trifluoro- 938-61-4, Benzene,
1,2,3,4-tetrachloro-5,6-difluoro- 1198-56-7, Benzene,
1,2,3,5-tetrachloro-4,6-difluoro- 1198-58-9, Benzene,
1,2,4,5-tetrachloro-3,6-difluoro- 1198-59-0, Benzene,
1,2-dichlorotetrafluoro- 1198-61-4, Benzene, 1,3-
dichlorotetrafluoro- 1198-62-5, Benzene, 1,4-dichlorotetrafluoro-
1422-93-1, 1,4-Cyclohexadiene, 1,2,4,5-tetrachloro-3,3,6,6-
tetrafluoro- 2712-78-9, Benzene, [bis(trifluoroacetoxy)iodo]-
3240-34-4, Benzene, (diacetoxyiodo)- 58776-08-2, Benzene,
(dinitratoiodo)- 75316-57-3, p-Cymene, 9-bromo- 89714-29-4,
Cyclohexane, heptachloropentafluoro- 89714-30-7,
Cyclohexene, hexachlorotetrafluoro- 89714-31-8,
Cyclohexane, hexachlorohexafluoro- 89714-32-9,

Cyclohexane, pentachloroheptafluoro- 89714-33-0, Cyclohexene, trichloroheptafluoro- 89714-34-1, Cyclohexene, tetrachlorohexafluoro- 89714-35-2, **Cyclohexane**, tetrachlorooctafluoro- 89714-36-3, **Cyclohexane**, trichlorononafluoro- 89799-46-2, Cyclohexene, pentachloropentafluoro- 91879-79-7, **Iodine**, oxobis(trifluoroacetato)diphenyldi- 95011-73-7, **Iodine**, oxobis(**hydrogen** sulfato)diphenyldi-
(**prepn.** of)

L57 ANSWER 19 OF 32 HCA

57:36606 Original Reference No. 57:7373b-i,7374a-f Preparation, resolution, and optical stability of 3,4-dehydroproline and 3,4-dehydroprolinamide. Robertson, Alexander V.; Witkop, Bernard (Natl. Insts. of Health, Bethesda, MD). Journal of the American Chemical Society, 84, 1697-1701 (Unavailable) **1962.**
CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 57:36606.

AB The redn. of pyrrole-2-carboxamide (I) with Ph4I in fuming HI under special conditions led to 70% 3,4-dehydro-DL-prolinamide (II) and 10% 3,4-dehydro-DL-proline (III), which were isolated and purified by ion exchange technique. The structures of DL-II and DL-III were proved by catalytic hydrogenation, nuclear magnetic resonance spectroscopy, and resolution. (All m.ps. were cor.). Pyrrole-2-carboxylie acid (IV) (Smissman, et al., CA 51,365d) was converted via its acid chloride into I. HI (57%, 250 ml.) satd. with HI (generated from 150 g. red P and 450 ml. 2:1 **iodine**-57% HI) at -20.degree. (Me2CO-dry ice bath), the soln stirred magnetically (no cooling bath) while adding quickly 25 g. crushed PH4I [Work, Inorg. Syn. 2, 141(1946)] and 45 g. powd. I, kept about 2 hrs. in a closed flask (the pressure of HI which was generated as the mixt. slowly warmed to room temp. must be maintained to obtain the best results; a greased heavy glass stopper was wired on tightly), when the complex dissolved the flask quickly cooled below 0.degree. the stopper removed, the contents poured onto an equal vol. of ice and H2O, the soln. evapd. at 1 mm. at 45.degree. (bath temp.) as rapidly as possible, the residual paste dissolved in 500 ml. H2O, the soln. chromatographed on 600 ml. Dowex 50W-X8 resin (**H+ form**), the column washed with H2O until the eluate was colorless, neutral, and free of iodide ion, eluted with 2N aq. NH3 until the eluate was colorless (700 ml.),the eluate evapd. in vacuo, the residue (36 g.) dried overnight in vacuo, and extd. 3 times with boiling abs. EtOH contg. 10% **C6H6** gave 4 g. (solvent-insol.) DL-III, m. 236-7.degree. (>10:2 EtOH-H2O); the combined exts. evapd., the residue (32 g.) chromatographed in H2O on 200 ml. Dowex 1-X8 (OH-form), the column washed with H2O (collecting eluate from the time it became alk. until it was again neutral), and the eluate evapd. gave DL-II, m. 95-6.degree. (**C6H6**), slowly becoming yellow on storage (succeeding elution

with 2N AcOH gave a small amt. of DL-III). DL-II and DL-III decolonized Br-H2O instantly and showed only end absorption in their ultraviolet spectra (in H2O). DL-III gave a yellow ninhydrin color and DL-II liberated NH3 in hot aq. NaOH. DL-II (1 g.) in 10 ml. cold EtOH treated with 1 ml. 10N HCl gave DL-II.HCl, m. 190-2.degree. (decompn.) (EtOH) DL-H (100 mg.) heated 2 hrs. on a steam bath in 5 ml. 5N HCl, evapd. in vacuo, the residue chromatographed on 5 ml. Dowex 50W (**H+ form**), the column washed with H2O until free of chloride ion, eluted with 20 ml. 2N aq. NH3, and the eluate evapd. gave DL-III, m. 236-7.degree. (H2O-EtOH). DL-III (100 mg.) in 2 ml. 2N HCl hydrogenated with 20 mg. PtO2 (1 molar equiv. H was rapidly absorbed), filtered, the filtrate percolated through 5 ml. Dowex 50W (**H+ form**), the column washed with H2O until free of chloride ion, eluted with 2N aq. NH3, the eluate evapd., and the residue recrystd. from MeOH-Et2O gave DL-proline. DL-II (50 mg.) in 5 ml. EtOH hydrogenated over 10 rag. PtO2 (rapid quant. H absorption), filtered, and the filtrate evapd. gave DL-prolinamide, m. 99.degree. (**C6H6-cyclohexane**). DL-II (28 g.) dissolved in 500 ml. H2O, the soln. adjusted to pH 8.0 with AcOH, combined with a soln. of hog kidney amidase (derived from 2 kg. hog kidney; the lyophilized enzyme prepn was dissolved in 300 ml. H2O contg. 2.0 g. MgCl2.6H2O and incubated 1 hr. at 38.degree.), made up to 1 l. H2O, incubated at pH 8.0 (this required periodic addn. of AcOH) (DL-II was 50% hydrolyzed after 25 hrs. and 60% after 43 hrs.), adjusted to pH 5 with AcOH, stirred with C, filtered, the filtrate chromatographed on 300 ml. Dowex 50W (**H + form**), the column washed with H2O until the washings were neutral and colorless, eluted with 2N aq. NH3, the eluate evapd., the residue dissolved in H2O, the soln. chromatographed on 300 ml. Dowex 1 (OH-form), the column washed with H2O (6 g. DL-II recovered), and eluted with 2N AcOH gave 17 g. L-III, m. 236-7.degree., [.alpha.]20D -375.degree. (H2O); attempts to increase the specific rotation of samples, [.alpha.]D >-370.degree. by recrystn. from H2O-EtOH failed. L-III (226 mg., [.alpha.]D -378.degree.) hydrogenated like DL-III and the aq. NH3 eluate evapd. gave L-proline, [.alpha.]20D -82.degree. (c 2, H2O). L-III, [.alpha.]20D -385.degree. (c 1, H2O), -257.degree. (c 1, 5N HCl), contained 3.degree./o D-III by manometric assay with D-amino acid oxidase. Oxidn. of L-III gave quant. IV, .lambda. 263 m.mu.. The optical activity of L-III in H2O (pH 6) at 20.degree. was unchanged after a week, but at 90.degree. the rotation decreased by 10%/day. Racemization of L-III was base-catalyzed, the half-life time at 20.degree. being 17 days at pH 11.5 and 9.5 days at pH 14. At 38.degree. and pH 8, the optical activity was decreased by 5% in 2 days and 10% in 4 days. L-III (165 mg., [.alpha.]D -256.degree.) in 8 ml. N NaOH heated 2 hrs. on a steam bath gave DL-III, m. 234 -6.degree. (H2O-Et2O). (+)-.alpha.-Bromocamphor-.pi.-sulfonic acid

(V) NH4 salt (21.2 g.) and 7.3 g. DL-II dissolved in a small vol. of H2O, the soln. evapd. several times in vacuo with small vols. MeOH, the residue dissolved in 200 ml. hot-EtOH, the soln. dild. with 200 ml. hot **C6H6**, concd. to half vol. by boiling, and kept overnight deposited 5.42 g. D-II.(+)-V, m. 240-2.degree. (EtOH-**C6H6**), [.alpha.]20D 160.degree. (c 2, H2O). D-II.(+)-V (4.23 g.) in 20 ml. H2O percolated through 50 ml. Dowex 1 (OH-form), the column washed with H2O, and the combined effluent and washings evapd. in vacuo as quickly as possible gave 1.067 g. D-II, [.alpha.]20D 300.degree. (c 2, H2O). Recrystn. of D-II ([.alpha.]20D 300.degree.) from **C6H6** gave D-II, [.alpha.]20D 260.degree.. The optical activity of D-II in H2O (pH 9.5) decreased at 20.degree. with a half-life time of 48 hrs. Aq. D-II heated 30 min. on a steam bath gave DL-II, m. 93-5.degree.. D-II (112 mg., [.alpha.]D 300.degree.) in 5 ml. EtOH and 2 ml. N HCl hydrogenated over 50 mg. PtO2 (quant. absorption of H occurred) gave L-prolinamide-HCl, [.alpha.]20D 59.degree. (c 2, EtOH). L-III at 0.5 p.p.m, still caused noticeable inhibition of growth in growing carrot phloem explant tissue cultures, and in this respect surpassed hydroxy-L-proline by a factor of 10. The reversible competitive inhibition was counteracted by L-proline. L-III was a powerful proline antimetabolite for several microorganisms. L-III added to the culture medium of Streptomyces antibioticus significantly changed the normal compn. (Katz and Goss, CA 53, 11505h) of the actinomycin complex in such a way that the biosynthesis of actinomyein II and III was favored. The implication of the principle of 100% conversion of a racemate into 1 natural optical isomer was discussed with regard to the origin of asymmetry in nature.

IT **74-85-1**, Ethylene
    (reactions of, with CBrCl3, explosion in)
RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

CC 38 (Amino Acids, Peptides, and Proteins)
IT **74-85-1**, Ethylene
    (reactions of, with CBrCl3, explosion in)

L57 ANSWER 20 OF 32 HCA COPYRIGHT 2006 ACS on STN
57:36409 Original Reference No. 57:7289h-i,7290c-i,7291a-i,7292a-i,7293a-f Solvated metalloorganic compounds. GroizeleauMiginiac, Leone (Univ. Paris, Paris, Fr.). Ann. Chim. (Paris), 6, 1071-1130 (Unavailable) **1961.** OTHER SOURCES: CASREACT 57:36409.

L57 ANSWER 21 OF 32 HCA COPYRIGHT 2006 ACS on STN

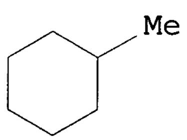
57:27651 Original Reference No. 57:5502i,5503a-b Radiolysis of methylcyclohexane. II. Liquid-phase inhibition by benzene. Freeman, G. R. (Univ. Alberta, Edmonton, Can.). Journal of Chemical Physics, 36, 1542-47 (Unavailable) **1962.** CODEN: JCPSA6. ISSN: 0021-9606.

AB The effect of **C6H6** on the radiolysis of liquid methylcyclohexane (I) was studied over the **C6H6** concn. range 0.25-100 mole %. The dominant effect of **C6H6** at low concns. is one of H atom scavenging. At higher concns., the transfer of energy (excitation or ionization) from activated I to **C6H6** also becomes important. As in the liquid **cyclohexane** system, there are 2 major reactive species in .gamma.-irradiated I. One species, C7H14', decomp. to **produce** cold **H** atoms that can be scavenged by **C6H6.** The other species, C7H14'' or C7H14+, **produces H** by a mechanism that is not subject to atom scavenging, but which can be inhibited by an energy transfer process. The 100-e.v. yields of the activated spp. in **pure I** are G(C7H14') = 1.8 .+-. 0.3 and G(C7H14) = 3.0 .+-. 0.3. These compare with the **cyclohexane** yields G(**C6H12** ') = 2.4 .+-. 0.3 and G(**C6H12**'') = 3.0 .+-. 0.3.

IT **108-87-2**, **Cyclohexane**, methyl-
(decompn. of, by .gamma.-rays, benzene effect on)

RN 108-87-2 HCA

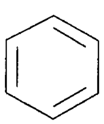
CN Cyclohexane, methyl- (8CI, 9CI) (CA INDEX NAME)



IT **71-43-2**, Benzene
(methylcyclohexane decompn. by .gamma.-rays in presence of)

RN 71-43-2 HCA

CN Benzene (8CI, 9CI) (CA INDEX NAME)



CC 11 (Radiation Chemistry and Photochemistry)

IT **108-87-2**, **Cyclohexane**, methyl-
(decompn. of, by .gamma.-rays, benzene effect on)

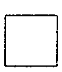
IT 1333-74-0, **Hydrogen**
(**formation** or evolution of, from methylcyclohexane by

.gamma.-rays, in presence of benzene)
IT **71-43-2**, Benzene
(methylcyclohexane decompn. by .gamma.-rays in presence of)

L57 ANSWER 22 OF 32 HCA COPYRIGHT 2006 ACS on STN
54:16752 Original Reference No. 54:3310b-i Experiments in the cyclobutane series. V. cis- and trans-1-(4-Dimethylamino-.alpha.-phenylbenzylidene)-2-(diphenylmethylene)cyclobutane. Kipping, F. B.; Wren, J. J. Journal of the Chemical Society 2465-73 (Unavailable) **1959.** CODEN: JCSOA9. ISSN: 0368-1769.
AB cf. C.A. 51, 17839d. In further attempts to demonstrate optical activity in the 1,2-bis(diphenylmethylene)cyclobutane system, the isomeric amines, cis- (I) and trans-1-(4-dimethylamino-.alpha.-phenylbenzylidene)-2-(diphenylmethylene)cyclobutane (II) were prepd. Heat, light, Al2O3, and acid facilitated their interconversion; acid surprisingly favored the I configuration. The UV spectra of these and related compds., particularly trans-trans-1-(p-dimethylaminophenyl)-4-phenyl-1,3-butadiene (III), were discussed. trans-trans-1,4-Diphenyl-1,3-butadiene (IV) was chromatographed and recrystd., m. 153-3.5.degree. (hexane). Crude III was a viscous red oil which gave only a few crystals after 3 wk. Its soln. in **C6H6** was extd. twice with concd. HCl. The combined exts. shaken with excess aq. NaOH and **C6H6**, the evapd., and the solid crystd. gave yellow plates. These plates chromatographed on Al2O3 gave pure III, m. 183.5-4.0.degree. (hexane). Solns. of III in CCl4 and hexane in the presence of air slowly decompd. In UV light crystals of III fluoresced intensely pale yellow-green, solns. in hexane pale blue, and those in alc., Me2CO, or CHCl3 pale yellow-green. For spectrophotometry, solns. of III were prepd. in the dark. III (17.5 mg.) in 75 mL. hexane was illuminated 8 h., the soln. evapd., and the residual oil chromatographed in CCl4 on a column of Al2O3. Simultaneously pure III (17.5 mg.) in an equal amt. of solvent was chromatographed on a 2nd column. Both columns were cut up and various fractions eluted with alc. These indicated that zone f of the first column contained cis-trans- and (or) trans-cis-amine, which yielded an oil which crystd. as the trans-trans-amine, .lambda. 368 m.mu.. p-Lithio-N,N-dimethylaniline in 70 mL. Et2O prepd. from 13.6 g. p-bromodimethylaniline and 0.95 g. Li, refluxed 0.5 h., 19.6 g. (.+-.)-1-benzoyl-2-(diphenylmethylene)cyclobutane in 40 mL. **C6H6** added, the soln. refluxed 0.5 **h.**, and the **product** steam distd. gave the (.+-.)-olefinic alc. (V), m. 158-8.5.degree. (alc.). Treatment of an Et2O soln. of crude V with dry HCl or aq. HCl gave a mixt. of the HCl salts of I and II. The whole amt. of V in CHCl3 shaken with dil. HCl, then with excess dil. NaOH, finally with H2O, and the CHCl3 soln. evapd. gave 15.7 g. mixed I and II, m. 141-50.degree.. Stored in the dark during 1 mo, the mother liquor deposited 3.5 g. almost pure II, yellow rods, m.p. depending upon

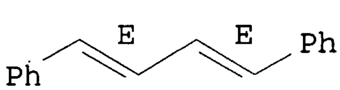
the rate of heating; placed in a bath at 181.degree. II m. 182-3.degree. (**cyclohexane**). I and II (10.5 g.) and 5.7 g. anhyd. (+)-camphor-10-sulfonic acid in 10 mL. **C6H6**, cooled, seeded, and left overnight gave 9.9 g. of the cis-(.+-.)-camphor-10-sulfonate (VI), m. 187.5-90.0.degree. (decompn.), [.alpha.]20D 17.8.degree. (c 2, **C6H6**). Using pure II also gave VI. VI shaken with excess aq. NaON and Et2O, the Et2O layer sepd., washed, and evapd. gave **pure I** ; when placed in a bath at 190.degree. it melted rapidly. VI showed no optical activity when 4% solns. were examd. in 4 dm. tubes. I in refluxing MeI cooled and left overnight gave I.MeI, m. 194-4.5.degree. (decompn.), pale green fluorescence in UV light. Similarly obtained was II.MeI, bluish rods, m. 205-6.degree. (decompn.). Ag (+)-camphor-10-sulfonate (580 mg.) and 974 mg. I.MeI each in 20 mL. MeOH gave 1.04 g. I-metho-(+)-camphor-10-sulfonate-3H2O (VII). VII evolved H2O at about 130.degree. and m. 180.degree.. Warmed with **C6H6** it gave an opalescent soln. which would not crystallize. The H2O of crystn. was removed to give a product, m. 212-13.degree.. All crops of VII had [.alpha.]21D 14.8.degree. (c 0.6, MeOH). When a soln. of the first crop was passed through Dowex 1 X-2 the eluate was optically inactive. By the same method a 79% yield of the metho-(+)-camphor-10-sulfonate of II was obtained, m. 263-5.degree. (decompn.), [.alpha.]22D 13.8.degree. (c 1.6, MeOH). Ion exchange carried out as above gave an optically inactive eluate.

IT **287-23-0**, Cyclobutane
(derivs.)
RN 287-23-0 HCA
CN Cyclobutane (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **538-81-8**, 1,3-Butadiene, 1,4-diphenyl-, trans-trans-
(prepn. of)
RN 538-81-8 HCA
CN Benzene, 1,1'-(1E,3E)-1,3-butadiene-1,4-diylbis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



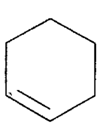
CC 10E (Organic Chemistry: Benzene Derivatives)
IT **287-23-0**, Cyclobutane 3144-16-9, 10-Camphorsulfonic acid,

d-
(derivs.)
IT **538-81-8**, 1,3-Butadiene, 1,4-diphenyl-, trans-trans-
82102-25-8, Aniline, N,N-dimethyl-p-4-phenyl-1,3-butadienyl-, trans,trans-
(prepn. of)

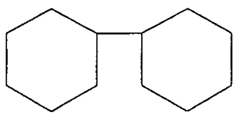
L57 ANSWER 23 OF 32 HCA COPYRIGHT 2006 ACS on STN
54:4931 Original Reference No. 54:1042h-i Radiation chemistry of organic compounds. IV. **Cyclohexane.** Dewhurst, Harold A. (Gen. Elec. Co., Schenectady, NY). Journal of Physical Chemistry, 63, 813-16 (Unavailable) **1959.** CODEN: JPCHAX. ISSN: 0022-3654.
AB cf. C.A. 53, 10999h. The major products formed in the 800-kv. peak electron radiolysis of **cyclohexane** are H, cyclohexene, and bicyclohexyl. Minor amts. of products result from fragmentation and isomerization of the ring system. The initial yields are G(C6H10) 2.5 and G(bicyclohexyl) 2.0 and were unchanged by irradiation either in 10 atm. of H or at liquid-N temp. In the presence of solutes, O, I, and benzene, the cyclohexene yield decreased to a limiting value of G = 0.7. The results were discussed in terms of a mechanism that involves the decompn. of excitedc yclohexane mols. Of the excited mols. that decomp., approx. 15% give products directly by an unspecified mol. process.
IT **7553-56-2**, **Iodine**
(effect on **cyclohexane** electron bombardment)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

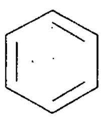
IT **110-83-8**, Cyclohexene
(formation of, from **cyclohexane** by electron bombardment)
RN 110-83-8 HCA
CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



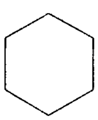
IT **92-51-3**, Bicyclohexyl
(formation of, in **cyclohexane** decompn. by electrons)
RN 92-51-3 HCA
CN 1,1'-Bicyclohexyl (9CI) (CA INDEX NAME)



IT **71-43-2**, Benzene
(in **cyclohexane** decompn. by electron bombardment)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



IT **110-82-7**, **Cyclohexane**
(radiolysis of, by electron bombardment)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 2 (General and Physical Chemistry)
IT Isomerization
(of **cyclohexane**, in decompn. by electron bombardment)
IT 183748-02-9, Electron
(**cyclohexane** bombardment by)
IT 7782-44-7, Oxygen
(effect on **cyclohexane** decompn. by electron bombardment)
IT **7553-56-2**, **Iodine**
(effect on **cyclohexane** electron bombardment)
IT **110-83-8**, Cyclohexene
(formation of, from **cyclohexane** by electron bombardment)
IT **92-51-3**, Bicyclohexyl
(formation of, in **cyclohexane** decompn. by electrons)
IT 1333-74-0, **Hydrogen**
(**formation** or evolution of, from **cyclohexane** by electrons)
IT **71-43-2**, Benzene

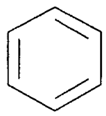
(in **cyclohexane** decompn. by electron bombardment)
IT **110-82-7, Cyclohexane**
(radiolysis of, by electron bombardment)

L57 ANSWER 24 OF 32 HCA COPYRIGHT 2006 ACS on STN
53:94496 Original Reference No. 53:16998b-i,16999a-i,17000a-c
Conformational analysis. V. The reaction of cis- and trans-4-tert-butylcyclohexanol and trans-4-methylcyclohexanol with phosphorus pentabromide. Syntheses of alkylcyclohexyl bromides.
Eliel, Ernest L.; Haber, Ralph G. (Univ. of Notre Dame, IN).
Journal of Organic Chemistry, 24, 143-51 (Unavailable) **1959**
. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT
53:94496.

L57 ANSWER 25 OF 32 HCA COPYRIGHT 2006 ACS on STN
53:87912 Original Reference No. 53:15788i,15789a-b **Hydrogen** iodide **production** in radiolysis of organic liquids containing dissolved **iodine**: **cyclohexane**, hexane, benzene. Meshitsuka, Gisuke; Burton, Milton (Univ. Notre Dame, Notre Dame, IN). Radiation Research, 10, 499-506 (Unavailable) **1959.** CODEN: RAREAE. ISSN: 0033-7587.
AB cf. C.A. 52, 19510d. Radiolysis of **cyclohexane** (I), hexane (II), and benzene (III) solns. contg. dissolved **I2** by Co60 .gamma.-rays produces HI. Initial yields, G(HI), are: I 2.1; II 2.5; III 0.9. The apparent yield of HI decreases with irradiation time and with postirradiation time. Low yields previously reported are attributed in part to rapid reactions of HI with intermediate irradiation products. [**I2**] concn. is varied from 0 to 0.025M, and [HI] concn. is varied from 0 to 0.0007M at const. [**I2**]. A brief discussion of the reaction kinetics is included.
IT **7553-56-2, Iodine**
(gamma-ray bombardment of org. solns. of, HI formation in)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

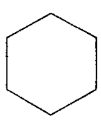
IT **71-43-2**, Benzene **110-54-3**, Hexane **110-82-7**
, **Cyclohexane**
(**iodine** solns. in, .gamma.-ray bombardment of, HI formation in)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

Me— $(CH_2)_4$—Me

RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



CC 3 (Electronic Phenomena and Spectra)
IT **7553-56-2, Iodine**
(gamma-ray bombardment of org. solns. of, HI formation in)
IT **71-43-2**, Benzene **110-54-3**, Hexane **110-82-7**
, Cyclohexane
(**iodine** solns. in, .gamma.-ray bombardment of, HI formation in)

L57 ANSWER 26 OF 32 HCA COPYRIGHT 2006 ACS on STN
53:72705 Original Reference No. 53:13192g-i,13193a-i,13194a-i,13195a-b Cyclane stereochemistry. XLIII. N-Menthones and their derivatives; racemic menthones and their derivatives. Laine, Francois; Lemoine, Hubert; Cornubert, Raymond (Univ. Nancy, Nancy, Fr.). Bulletin de la Societe Chimique de France 1346-52 (French) **1958.** CODEN: BSCFAS. ISSN: 0037-8968. OTHER SOURCES: CASREACT 53:72705.

L57 ANSWER 27 OF 32 HCA COPYRIGHT 2006 ACS on STN
52:110558 Original Reference No. 52:19510d-g Radiation protection in **cyclohexane.** Burton, M.; Chang, J.; Lipsky, S.; Reddy, M. P. (Univ. of Notre Dame, Notre Dame, IN). Radiation Research, 8, 203-13 (Unavailable) **1958.** CODEN: RAREAE. ISSN: 0033-7587.
AB The effects of low concns. of **iodine**, bromobenzene, MeI, EtI, benzene, and cyclohexyl iodide on $G(H_2)$ for irradiated **cyclohexane**(I) are given. The effects of benzene on the **cyclohexane-iodine** system are also described and

interpreted. The solns. were irradiated by Co60 .gamma.-rays at a dosage rate of about 2 .times. 1019 e.v./l./min. H is the principal gaseous product. With **iodine** added to I G(H2) drops from 5.85 to 3.8 at **iodine** concns. of 0.01-0.03M. A plateau is assumed in the G(H2) vs. **iodine** concn. curve. No such plateau is found for I irradiated in the presence of benzene or the other alkyl and aromatic iodides. In the system I-0.03M **iodine**, added benzene increases G(H2) from 3.6 to a max. of 4.05 at 0.01M **C6H6**; G(H2) decreases rapidly at higher **C6H6** concns. Replacement of **C6H6** by C6D6 shows no D in the H. No such max. is found in the I-**C6H6** system. About 10% of G(H2) remains at infinite relative **C6H6** concn. and at high **iodine** concn. The H yields are explained by (a) a mol. process involving **C6H12** .fwdarw. C6H10 + H2 with no radical intermediates and (b) the conversion of an excited I into some **form** yielding **H** and a cyclohexyl radical.

IT **110-54-3**, Hexane **112-40-3**, Dodecane **124-18-5**, Decane **142-82-5**, Heptane
(decompn. by .gamma.-rays)

RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-Me$

RN 112-40-3 HCA
CN Dodecane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_{10}-Me$

RN 124-18-5 HCA
CN Decane (8CI, 9CI) (CA INDEX NAME)

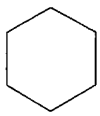
$Me-(CH_2)_8-Me$

RN 142-82-5 HCA
CN Heptane (8CI, 9CI) (CA INDEX NAME)

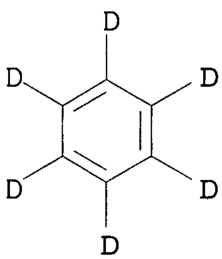
$Me-(CH_2)_5-Me$

IT **110-82-7**, **Cyclohexane**
(decompn. of, by .gamma.-rays)

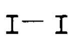
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



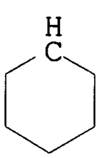
IT **1076-43-3**, Benzene-d6
(effect on **cyclohexane** decompn. by .gamma.-rays)
RN 1076-43-3 HCA
CN Benzene-d6 (8CI, 9CI) (CA INDEX NAME)



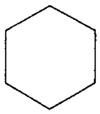
IT **7553-56-2, Iodine**
(effect on **cyclohexane** .gamma.-ray bombardment)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)



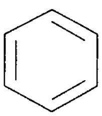
IT **3170-58-9**, Cyclohexyl
(formation in **cyclohexane** .gamma.-ray bombardment)
RN 3170-58-9 HCA
CN Cyclohexyl (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **110-82-7, Cyclohexane**
(gamma-ray bombardment of, protective agents in)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT 71-43-2, Benzene
(in **cyclohexane** decompn. by .gamma.-rays)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



IT **111-65-9**, Octane
(isomers, decompn. by .gamma.-rays)
RN 111-65-9 HCA
CN Octane (8CI, 9CI) (CA INDEX NAME)

Me— $(CH_2)_6$—Me

CC 3 (Electronic Phenomena and Spectra)
IT Gamma rays
(**cyclohexane** bombardment by, protective agents in)
IT **110-54-3**, Hexane **112-40-3**, Dodecane
124-18-5, Decane **142-82-5**, Heptane
(decompn. by .gamma.-rays)
IT **110-82-7**, **Cyclohexane**
(decompn. of, by .gamma.-rays)
IT 74-88-4, Methane, iodo- 75-03-6, Ethane, iodo- 108-86-1,
Benzene, bromo- 626-62-0, **Cyclohexane**, iodo-
1076-43-3, Benzene-d6
(effect on **cyclohexane** decompn. by .gamma.-rays)
IT **7553-56-2**, **Iodine**
(effect on **cyclohexane** .gamma.-ray bombardment)
IT **3170-58-9**, Cyclohexyl
(formation in **cyclohexane** .gamma.-ray bombardment)
IT 1333-74-0, **Hydrogen**
(**formation** or evolution of, from **cyclohexane**
by .gamma.-rays)
IT **110-82-7**, **Cyclohexane**
(gamma-ray bombardment of, protective agents in)
IT **71-43-2**, Benzene

(in **cyclohexane** decompn. by .gamma.-rays)
IT **111-65-9**, Octane
(isomers, decompn. by .gamma.-rays)

L57 ANSWER 28 OF 32 HCA COPYRIGHT 2006 ACS on STN
52:50526 Original Reference No. 52:9067f-i,9068a-h Decomposition reactions of heterocyclic diacyl peroxides. II. 2-Thenoyl peroxide. Ford, M. C.; Mackay, Donald (Univ. Old Aberdeen, UK). Journal of the Chemical Society 4620-5 (Unavailable) **1957.** CODEN: JCSOA9. ISSN: 0368-1769.
AB cf. C.A. 45, 9027h. Compds. formed by the decompn. of 2-thenoyl peroxide (I) in aromatic solvents can be attributed largely to reactions of 2-thenoyloxy radicals. The most regular feature was the formation of aryl 2-thenoates, in low yield, by nuclear attack, and in the halobenzenes phenyl 2-thenoate (II) was formed, with displacement of the halogen. In PhMe and cumene (III) attack occurred preferentially in the side chain. In solvents lacking side chain **H**, the **formation** of 2-thenoic anhydride (IV) was sometimes observed. In thiophene (V), 2-thienyl 2-thenoate (VI) and 2,2'-bi-thienyl (VII) were produced, VII providing evidence for the generation of 2-thienyl radicals. 2-Thenoic acid (VIII), m. 127-8.degree., with SOCl2 gave a nearly quant. yield of the acid chloride (IX), b10 77.degree.. The following esters of VIII were prepd. under Schotten-Baumann conditions from the appropriate phenol: II, m. 54.degree.; 1-naphthyl (X), m. 80.degree.; p-ClC6H4 (XI), m. 84-4.5.degree.; p-BrC6H4 (XII), m. 85.degree.; VI, m. 54.degree.; p-O2NC6H4, (XIII), m. 181.degree. (MeOH). IX (14 g.) in 20 ml. **cyclohexane** stirred 20 min. with 40 ml. 2N NaOH and 50 ml. 30-vol. H2O2 gave 60-5% I, prisms, m. 103.degree. (**C6H6**-ligroine). The decompns. of I in **C6H6**, the halobenzenes, and nitrobenzenes were carried out in the dark, and on an oil bath. Working up consisted in removal of the solvent in vacuo, extn. with Et2O, and sepn. of the acid by repeated shaking with 2N KHCO3. Except in the case of the PhMe decompn., the acid was obtained pure after recrystn. from H2O. After drying of the Et2O soln. the solvent was removed and the neutral residue treated as described. I (6.0 g.) decompd. in 600 ml. **C6H6** 48 hrs. at 75-85.degree. under N evolved 0.26 mole CO2; the solvent removed, and the resulting tar extd. with Et2O gave 1.9 g. VIII and neutral material which, distd. at 0.01 mm., yielded 0.7 g. of an oil, and chromatography on anhyd. MgSO4 gave 0.2 g. II, m. 53.degree. and 0.3 g. IV, m. 60.5-1.5.degree. (ligroine). In another expt. 750 mg. I decompd. during 24 hrs. in 75 ml. **C6H6**, the solvent removed through a short column, and the distillate tested with isatin in concd. H2SO4 showed that the mixt. contained 1 mg. V. I (1.0 g.) heated 10 hrs. at 80-90.degree. with 20 g. C10H8 in 20 ml. **C6H6** gave 0.54 g. VIII and 0.1 g. X. Decompn. of 12 g. I in 1180 ml. PhNO2 36 hrs. at 85-95.degree. similarly gave 2.7 g. VIII

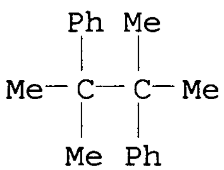
and 50 mg. crude XIII. I (18 g.) heated 45 hrs. at 65-75.degree. in 1620 ml. PhCl and the neutral material distd. at 0.01 mm. chromatography on MgSO4 gave 1.4 g. material which, rechromatographed on Norit, yielded 0.38 g. II, 0.02 g. XI, and 0.17 g. VI. The 2nd fraction of 1.4 g. rechromatographed on MgSO4 from ligroine gave IV, m. 59.5.degree. (ligroine). In a similar expt., in which 9 g. I gave 0.24 g. II, the total combined Cl was found to amt. 0.11 g. I (15 g.) decompd. 24 hrs. at 75-80.degree. in 1400 ml. PhBr, distd., and chromatographed on Norit gave 0.17 g. II and 0.26 g. XII. I (7 g.) in 100 ml. PhBr added during 3 hrs. to 500 ml. PhBr under reflux with the effluent gases passed through acidified AgNO3 and refluxed a further hr. gave 2.1 millimoles AgBr and 2.6 g. VIII, 0.57 g. II, and a trace of XII. I (2.5 g.) in 60 ml. PhI added all at once to 190 ml. PhI at 150.degree., and the whole heated 5 min. at 150.degree. gave 0.9 g. VIII, 0.12 g. II, and 30 mg. IV. The liberated **iodine** was extd. with satd. aq. KI and titrated with 0.1N thiosulfate. I (18 g.) decompd. 48 hrs. at 75-85.degree. in 1700 ml. PhMe gave 12.5 g. acidic material shown to contain 11 g. pure VIII. Trituration of the insol. fraction gave 0.17 g. 5(?)-(2-thenoyloxy)-2-thenoic acid (XIV), prisms, m. 195.degree. (decompn.). XIV with CH2N2 gave the Me ester, m. 131-2.degree. (decompn.)(ligroine). XIV on hydrolysis gave VIII, together with a highly sol. hydroxythenoic acid, which with aq. FeCl3 formed an intense vermilion color, rapidly changing to a dark red ppt. The residue from the org. layer gave 4.5 g. material, b0.01 70-80.degree., which on recrystn. yielded Ph2, m. 48-50.degree., and the mother liquor evapd. and the residue chromatographed on Al2O3 gave 2.9 g. more Ph2 and 2-benzylthiophene (XV) characterized by conversion to 2-benzyl-5-(chloromercuri)thiophene, prisms, m. 184-5.degree. (MeOH-CHCl3). The 2nd fraction (1.5 g.) refluxed 0.5 hr. with 4 g. KOH in 25 ml. alc., the alc. removed, H2O added, and the soln. extd. with Et2O gave 0.4 g. PhCH2OH; phenylcarbamate, m. 76-7.degree.. The alk. soln. gave 0.7 g. VIII and 0.2 g. phenolic material, which with 1-C10H7NCS yielded .omicron.-tolyl .alpha.-naphthylcarbamate, m. 136.degree.. In another expt. (1 g. I in 95 ml. PhMe) the effluent N was passed through a trap at -70.degree. and the solvent distd., giving about 0.2 mg. V. I (3.0 g.) in 300 ml. III 36 hrs. at 70-80.degree. gave 3 g. VIII and 0.24 g. (Me2CPh)2, m. 117.degree. (MeOH). I (3.0 g.) in 100 ml. V refluxed 16 hrs. gave 1.3 g. VIII, and distn. of the org. fraction yielded 0.50 g. VI. The ligroine-sol. fraction chromatographed on MgSO4 yielded 0.12 g. VII, m. 34-5.degree., and 0.73 g. more VI. Bz2O2 (4.0 g.) in 100 ml. V refluxed 24 hrs. and similarly worked up gave 2.6 g. BzOH and 0.51 g. 2-thienyl benzoate, m. 43-4.degree.. I (3 g.) added in small portions to 6 g. Et2S and refluxed 3 min. after the exothermic reaction had occurred gave 1.9 g. VIII and 0.63 g. IV. Similarly 8 g. Bz2O2 with 16 g. Et2S gave 5 g. BzOH and 1.3 g. Bz2O. In neither

case was any attempt made to isolate the oxidation products of the sulfide. (tert-BuO)2 (10 g.), 50 ml. PhMe, and 50 ml. V refluxed 7 days and concd. gave a high-boiling residue which, extd. with ligroine, yielded 0.5 g. XV. No (PhCH2)2 was formed.

IT **1889-67-4**, Bibenzyl, .alpha.,.alpha.,.alpha.',.alpha.'-tetramethyl-
(prepn. of)

RN 1889-67-4 HCA

CN Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 527-72-0, 2-Thiophenecarboxylic acid **1889-67-4**, Bibenzyl, .alpha.,.alpha.,.alpha.',.alpha.'-tetramethyl- 3441-41-6, Phenol, p-chloro-, 2-thiophenecarboxylate 5271-67-0, 2-Thiophenecarbonyl chloride 13132-15-5, Thiophene, 2-benzyl- 25569-97-5, 2-Thiophenecarboxylic anhydride 38253-98-4, 1-Naphthol, 2-thiophenecarboxylate 91059-63-1, Phenol, p-nitro-, 2-thiophenecarboxylate 91635-19-7, Phenol, p-bromo-, 2-thiophenecarboxylate 99852-09-2, Thiophene, 2-benzyl-5-(chloromercuri)- 102028-25-1, 1-Naphthalenecarbamic acid, o-tolyl ester
(prepn. of)

L57 ANSWER 29 OF 32 HCA COPYRIGHT 2006 ACS on STN

49:42823 Original Reference No. 49:8210b-i,8211a-i,8212a-i,8213a-b
Synthetic estrogenic compounds related to stilbene and diphenylethane. III. Dodds, E. C.; Huang, R. L.; Lawson, W.; Robinson, Robert Proc. Roy. Soc. (London), B140, 470-97 (Unavailable) **1953.**

L57 ANSWER 30 OF 32 HCA COPYRIGHT 2006 ACS on STN

49:1254 Original Reference No. 49:268i,269a-i,270a-i,271a-i,272a-i,273a-i,274a-i,275a-f Terramycin. X. The structure of Terramycin. Hochstein, F. A.; Stephens, C. R.; Conover, L. H.; Regna, P. P.; Pasternack, R.; Gordon, P. N.; Pilgrim, F. J.; Brunings, K. J.; Woodward, R. B. (Harvard Univ.). Journal of the American Chemical Society, 75, 5455-75 (Unavailable) **1953.** CODEN: JACSAT. ISSN: 0002-7863.

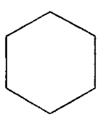
GI For diagram(s), see printed CA Issue.

L57 ANSWER 31 OF 32 HCA COPYRIGHT 2006 ACS on STN
41:31096 Original Reference No. 41:6246i,6247a-i,6248a-i,6249a-i,6250a-i,6251a-i,6252a-i,6253a-i,6254a-b The synthesis of analgesic compounds. Lee, John; Ziering, Albert; Berger, Leo; Heineman, Stephen D. (Hoffmann-La Roche Inc., Nutley, NJ). Jubilee Vol. Emil Barell 264-305 (English) **1946.**
GI For diagram(s), see printed CA Issue.

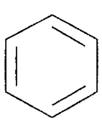
L57 ANSWER 32 OF 32 HCA COPYRIGHT 2006 ACS on STN
41:26516 Original Reference No. 41:5289g-i,5290a-d Conversion of hydrocarbons on aluminosilicate catalysts. I. **Cyclohexane.** Maslyanskii, G. N.; Berlin, T. S. (Central Research Inst. Aviation Fuels, Moscow). Zhurnal Obshchei Khimii, 16, 1643-54 (Russian) **1946.** CODEN: ZOKHA4. ISSN: 0044-460X.
AB In 1-hr. expts. over an artificial granulated aluminosilicate catalyst (SiO2 90, Al2O3 10%), vol. 50 ml., rate of flow r of **cyclohexane** 49.8 ml./hr., at 515.degree., the yield in catalyzate Y was 89.4 wt. %, gas 1300 ml. of the compn. (vol. %) CO2 0.4, H2 41.0, CnH2n 17.0, CnH2n+2 41.6; at the same temp., r 15.0, Y = 78.5%, amt. and compn. of gas almost unchanged; at 560.degree., Y = 62.2%, gas 3600 ml., of very nearly the same compn. as before. Typical fractionation of a catalyzate (515.degree., r 15 ml./hr.; **iodine** no. 5.9): b. >60, 60-75, 75-85, 85-100, 100-120, 120-150, > 150.degree.; 0.3, 11.2, 73.2, 0.6, 0.8, 1.0, 7.0 wt. %. By the ns and reaction with KMnO4, the 100-120.degree. and 120-150.degree. fractions contained mainly C6H5CH3 and C6H4(CH3)2, resp.; by the **iodine** no. and sulfonation, the **C6H6** and the unsatd. hydrocarbon content in the 60-75.degree. fraction constituted about 8% each; after hydrogenation, dehydrogenation and sulfonation, that fraction (by the aniline point) consisted of methylcyclopentane 76, hexanes 26; this indicates some amt. of isomerization of the **cyclohexane**; in the 75-85.degree. fraction, **C6H6** and unsatd. hydrocarbons constituted only about 1% each. Thus, formation of unsatd. hydrocarbons and simple dehydrogenation of **cyclohexane** into **C6H6** are only relatively slight at 515.degree., somewhat higher at 560.degree.: the fractions b. 60-75, 75-85, 85-100, 100-120, 120-150.degree.; 8.9, 62.6, 2.7, 3.6, 4.9%, resp., had the following contents in unsatd. and aromatic hydrocarbons: 14.1, 23.6; 2.0, 5.0; 2.5, 13.4; 0.0, 74.0; 0.0, .apprx. 100%; in the combined fractions 60-150.degree., **C6H6**, C6H5CH3, C6H4(CH3)2 and C6H5C2H5, aromatic compds. b. above 150.degree. constituted 5.6, 2.7, 4.9, 8.3%, resp. The main trend of the reaction is dehydrogenation of **cyclohexane** coupled with synthesis of alkyl-substituted **C6H6** derivs., by a mechanism thought to involve CH2 radicals. That the substitutions occur freely, especially at high temp., follows from the standard free energies at 833.degree.K., computed for the reactions: **C6H6** + n-C5H12 = C6H5CH3 +

n-C4H10, -7120; **C6H6** + n-C6H14 = C6H5CH3 + n-C5H12, -2830; C6H5CH3 + n-C5H12 = C6H4(CH3)2 + n-C4H10, -3260; **C6H6** + n-C5H12 = C6H5C2H5 + C3H8, -6030 cal./mole. Comparison of the amt. of H2 in the gas and the amt. of **C6H6** derivs. **formed** shows the **H2** to be in excess (up to 30%) of the stoichiometric ratio; this parallels the formation of high-C deposits on the catalyst which requires regeneration by an air stream at 510-540.degree. for 2 hrs.

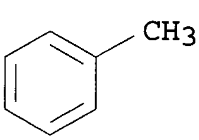
IT **110-82-7**, **Cyclohexane**
(reactions of, on aluminosilicate catalysts)
RN 110-82-7 HCA
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



IT **71-43-2**, Benzene
(reactions of, with C5H12 or C6H14, free energies of)
RN 71-43-2 HCA
CN Benzene (8CI, 9CI) (CA INDEX NAME)



IT **108-88-3**, Toluene
(reactions of, with C5H12, free energy of)
RN 108-88-3 HCA
CN Benzene, methyl- (9CI) (CA INDEX NAME)



IT **109-66-0**, Pentane
(reactions of, with benzene or toluene, free energies of)
RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

IT **110-54-3**, Hexane
(reactions of, with benzene, free energy of)
RN 110-54-3 HCA
CN Hexane (8CI, 9CI) (CA INDEX NAME)

$Me-(CH_2)_4-Me$

CC 22 (Petroleum, Lubricants, and Asphalt)
IT Energy
(free, of **C6H6** reaction with C5H12 or hexane and of C5H12 reaction with toluene)
IT Dehydrogenation
Isomerization
(of **cyclohexane**, on aluminosilicate catalysts)
IT **110-82-7**, **Cyclohexane**
(reactions of, on aluminosilicate catalysts)
IT **71-43-2**, Benzene
(reactions of, with C5H12 or C6H14, free energies of)
IT **108-88-3**, Toluene
(reactions of, with C5H12, free energy of)
IT **109-66-0**, Pentane
(reactions of, with benzene or toluene, free energies of)
IT **110-54-3**, Hexane
(reactions of, with benzene, free energy of)

=> d l58 1-22 cbib abs hitstr hitind

L58 ANSWER 1 OF 22 HCA COPYRIGHT 2006 ACS on STN
137:235061 In-situ hydrogasification of coal beds for methane production using steam-based iron oxidation for **hydrogen generation.** Kindig, J. Kelly; Odle, Robert R.; Weyand, Thomas E.; Davis, Boyd R. (USA). U.S. Pat. Appl. Publ. US 2002124466 A1 **20020912**, 15 pp. (English). CODEN: USXXCO. APPLICATION: US 2001-800421 20010306.
AB Coal, esp. low-grade coal contg. .gtoreq.2 wt.% S, is hydrogasified in-situ in the presence of a high-hydrogen reducing gas contg. carbon monoxide and >40 vol.% (preferably 99 vol.%) H2 at 700-900.degree., to produce CH4 and a **purified** (**i**.e., desulfurized) carbon-contg. byproduct. The reducing gas is produced as part of a steam oxidn. cycle of an active metal (e.g., Fe or Sn), in which the initial steam oxidn. of the metal **produces H2** and a metal oxide, which is then reduced by CO to regenerate the metal. A portion of the methane product can be burned in a combined-cycle process to provide electricity and power.

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IT   1333-74-0P, Hydrogen, preparation
        (generation of and coal hydrogasification with; in-situ
        hydrogasification of coal beds for methane prodn. using
        steam-based iron oxidn. for hydrogen generation
        )
RN   1333-74-0  HCA
CN   Hydrogen (8CI, 9CI)  (CA INDEX NAME)

H—H

IT   74-82-8P, Methane, preparation
        (manuf. of; in-situ hydrogasification of coal beds for methane
        prodn. using steam-based iron oxidn. for hydrogen
        generation)
RN   74-82-8  HCA
CN   Methane (8CI, 9CI)  (CA INDEX NAME)

CH4

IC   ICM  C10B057-04
INCL 048127300
CC   51-20 (Fossil Fuels, Derivatives, and Related Products)
     Section cross-reference(s): 49
IT   Coke
        (byproduct, in-situ formation of; in-situ hydrogasification of
        coal beds for methane prodn. using steam-based iron oxidn. for
        hydrogen generation)
IT   Coal gasification
        (hydrogasification; in-situ hydrogasification of coal beds for
        methane prodn. using steam-based iron oxidn. for hydrogen
        generation)
IT   Oxidation
        (of iron or tin, steam-mediated; in-situ hydrogasification of
        coal beds for methane prodn. using steam-based iron oxidn. for
        hydrogen generation)
IT   Steam
        (oxidn. with, of iron or tin; in-situ hydrogasification of coal
        beds for methane prodn. using steam-based iron oxidn. for
        hydrogen generation)
IT   7440-44-0P, Carbon, preparation
        (byproduct, in-situ formation of; in-situ hydrogasification of
        coal beds for methane prodn. using steam-based iron oxidn. for
        hydrogen generation)
IT   1345-25-1, Ferrous oxide, reactions   18282-10-5, Tin dioxide
        (carbon monoxide redn. of; in-situ hydrogasification of coal beds
        for methane prodn. using steam-based iron oxidn. for
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hydrogen generation)

IT **1333-74-0P, Hydrogen, preparation**
(**generation** of and coal hydrogasification with; in-situ hydrogasification of coal beds for methane prodn. using steam-based iron oxidn. for **hydrogen generation**
)

IT **74-82-8P**, Methane, preparation
(manuf. of; in-situ hydrogasification of coal beds for methane prodn. using steam-based iron oxidn. for **hydrogen generation**)

IT 630-08-0, Carbon monoxide, reactions
(reducing agent; in-situ hydrogasification of coal beds for methane prodn. using steam-based iron oxidn. for **hydrogen generation**)

IT 7439-89-6, Iron, processes 7440-31-5, Tin, processes
(steam oxidn. of; in-situ hydrogasification of coal beds for methane prodn. using steam-based iron oxidn. for **hydrogen generation**)

L58 ANSWER 2 OF 22 HCA COPYRIGHT 2006 ACS on STN

132:122273 The carbonylation of methanol catalyzed by [RhI(CO)(PEt3)2]; crystal and molecular structure of [RhMeI2(CO)(PEt3)2]. Rankin, Joanne; Benyei, Attila C.; Poole, Andrew D.; Cole-Hamilton, David J. (School of Chemistry, University of St. Andrews, St. Andrews, KY16 9ST, UK). Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (21), 3771-3782 (English) **1999.** CODEN: JCDTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

AB [RhCl(CO)(PEt3)2] catalyzes the carbonylation of methanol in the presence of MeI and water at a rate 1.8 times that for [RhI2(CO)2]- at 150 .degree.C. The reaction is first order in [MeI] and zero order in pCO. However, the phosphine complex degrades to [Rh(CO)2I2]- during the course of the reaction. Stoichiometric studies show that the rate of oxidative addn. of MeI to [RhI(CO)(PEt3)2] is 57 times faster than to [RhI2(CO)2]- at 298 K and that [RhMeI2(CO)(PEt3)2] can be isolated and crystallog. characterized. Combination of the Me and carbonyl ligands to give the acyl intermediate occurs 38 times slower for [RhMeI2(CO)(PEt3)2] than for [RhMeI3(CO)2]- but the steady state concn. of the intermediates is different in that [Rh(COMe)**I2**(PEt3)2] is thermodynamically less stable than [RhMeI2(CO)(PEt3)2]. In CH2Cl2, [Rh(COMe)**I2**(CO)(PEt3)2] reductively eliminates MeCOI. [RhI(CO)(PEt3)2] reacts with CO to give [RhI(CO)2(PEt3)2]. Catalyst degrdn. occurs via [RhHI2(CO)(PEt3)2], formed by oxidative addn. of HI to [RhI(CO)(PEt3)2], which reacts further with HI to give [RhI3(CO)(PEt3)2] from which [Et3PI]+ reductively eliminates and is hydrolyzed to give Et3PO. In the presence of water, much less [RhI3(CO)(PEt3)2] and Et3PO are formed so the catalyst is more

stable, but loss of [Et3PMe]+ and [Et3PH]+ from [RhMeI2(CO)(PEt3)2] or [RhHI2(CO)(PEt3)2], resp., lead to catalyst deactivation. The rate detg. step of the catalytic reaction in the presence of water is MeI oxidative addn. to [RhI(CO)(PEt3)2], but in the absence of water there is evidence that it may be reductive elimination of MeCOI from [Rh(COMe)**I2**(CO)(PEt3)2]. [RhMeI2(CO)(PEt3)2] has mutually trans phosphines and the Me group trans to I.

IT **74-82-8P**, Methane, preparation **1333-74-0P**, **Hydrogen, preparation**
(kinetics and mechanism of carbonylation of methanol catalyzed by [RhI(CO)(PEt3)2] and crystal and mol. structure of the catalytic species [RhMeI2(CO)(PEt3)2])

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 22-13 (Physical Organic Chemistry)
Section cross-reference(s): 45, 67, 75

IT **74-82-8P**, Methane, preparation 75-03-6P, Iodoethane 75-07-0P, Ethanal, preparation 79-09-4P, Propanoic acid, preparation 115-10-6P, Dimethyl ether 124-38-9P, Carbon dioxide, preparation 141-78-6P, Ethyl ethanoate, preparation **1333-74-0P**, **Hydrogen, preparation**
(kinetics and mechanism of carbonylation of methanol catalyzed by [RhI(CO)(PEt3)2] and crystal and mol. structure of the catalytic species [RhMeI2(CO)(PEt3)2])

L58 ANSWER 3 OF 22 HCA COPYRIGHT 2006 ACS on STN

125:119390 Thermal plasma pyrolysis of used old tires for production of syngas. Chang, J. S.; Gu, B. W.; Looy, P. C.; Chu, F. Y.; Simpson, C. J. (Dep. Eng. Physics, McMaster Univ., Hamilton, ON, L8S 4M1, Can.). Journal of Environmental Science and Health, Part A: Environmental Science and Engineering & Toxic and Hazardous Substance Control, A31(7), 1781-1799 (English) **1996.** CODEN: JESHE6. ISSN: 1077-1204. Publisher: Dekker.

AB Thermal plasma pyrolysis of used tires for the prodn. of syngas was investigated exptl. A series of expts. have shown that tire waste can be pyrolyzed in a plasma reactor to produce combustible gas, such as C2H2, CH4, C2H4, H2, CO. The combustion heat value of the produced gas is about 4-7 MJ/m3, which is higher than that of blast

furnace gas and reforming gas from coals. Zinc oxide can be captured during pyrolysis by both high temp. filters and low temp. filters in the quenching chamber. The pollutant gases, such as SO2 and NOx, are at relatively low levels, about 100-300 ppm. Increasing the tire injection quantity will increase the concn. of hydrocarbons, increase the combustion heat of the pyrolysis product, and decrease the concn. of metal oxide. With steam injection, it produced a large quantity of hydrogen and carbon monoxide with lower concns. of C2H2. The combustion heat is slightly lower with steam injection than that without it. Neither polychlorinated biphenyls nor p-aminohippuric acid were detected in the ashes.

IT **7553-56-2, Iodine,** formation (nonpreparative)
(pollutants, in pyro.iota.yzed ashes; thermal plasma pyrolysis of used old tires for prodn. of syngas)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **74-82-8P**, Methane, preparation **74-85-1P**, Ethylene, preparation **74-86-2P**, Acetylene, preparation **1333-74-0P, Hydrogen, preparation**
(thermal plasma pyrolysis of used old tires for prodn. of syngas)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-85-1 HCA

CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 74-86-2 HCA

CN Ethyne (9CI) (CA INDEX NAME)

$HC{\equiv}CH$

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 52-1 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 39, 60

IT 7429-91-6, Dysprosium, formation (nonpreparative) 7439-91-0, Lanthanum, formation (nonpreparative) 7439-95-4, Magnesium, formation (nonpreparative) 7439-96-5, Manganese, formation (nonpreparative) 7439-98-7, Molybdenum, formation (nonpreparative) 7440-00-8, Neodymium, formation (nonpreparative) 7440-09-7, Potassium, formation (nonpreparative) 7440-17-7, Rubidium, formation (nonpreparative) 7440-19-9, Samarium, formation (nonpreparative) 7440-23-5, Sodium, formation (nonpreparative) 7440-32-6, Titanium, formation (nonpreparative) 7440-33-7, Tungsten, formation (nonpreparative) 7440-36-0, Antimony, formation (nonpreparative) 7440-38-2, Arsenic, formation (nonpreparative) 7440-39-3, Barium, formation (nonpreparative) 7440-42-8, Boron, formation (nonpreparative) 7440-47-3, Chromium, formation (nonpreparative) 7440-48-4, Cobalt, formation (nonpreparative) 7440-55-3, Gallium, formation (nonpreparative) 7440-62-2, Vanadium, formation (nonpreparative) 7440-66-6, Zinc, formation (nonpreparative) **7553-56-2**, **Iodine**, formation (nonpreparative) 7704-34-9, Sulfur, formation (nonpreparative) 7726-95-6, Bromine, formation (nonpreparative) 7782-50-5, Chlorine, formation (nonpreparative)
(pollutants, in pyro.iota.yzed ashes; thermal plasma pyrolysis of used old tires for prodn. of syngas)

IT **74-82-8P**, Methane, preparation **74-85-1P**, Ethylene, preparation **74-86-2P**, Acetylene, preparation 124-38-9P, Carbon dioxide, preparation 630-08-0P, Carbon monoxide, preparation **1333-74-0P**, **Hydrogen**, **preparation**
(thermal plasma pyrolysis of used old tires for prodn. of syngas)

L58 ANSWER 4 OF 22 HCA COPYRIGHT 2006 ACS on STN

123:324269 Deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal in reprocessing plant. Wei, Y.-Z.; Takeshita, K.; Shimizu, M.; Kumagai, M.; Takashima, Y.; Matsumoto, S. (Nucl. Chem. Chem. Eng. Cent., Inst. Res. Innovation, Chiba, 277, Japan). Fusion Technology, 28(3, Pt. 2), 1585-90 (English) **1995.** CODEN: FUSTE8. ISSN: 0748-1896. Publisher: American Nuclear Society.

AB Deactivation of a hydrophobic Pt/SDBC catalyst for the H2/HTO isotopic exchange reaction used to remove T from the wastewater generated in a nuclear fuel reprocessing plant was studied exptl. The catalyst was poisoned reversibly by a small amt. of HNO3 and could be regenerated by washing with water followed by drying in an inert gas. As a countermeasure against this poisoning, the neutralization of the wastewater was found to be effective. The presence of **I2** in the wastewater caused a sharp decrease in the activity of the catalyst owing to the irreversible adsorption

of **I2** onto the catalyst surface. The **I2** poisoning could be prevented by the conversion of **I2** into I- or IO3- by neutralization or redox reaction. TBP and the neutral nitrate salts of fission products such as Sr(NO3)2 showed negligible poisoning effects on the catalyst.

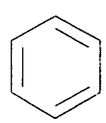
IT **9003-70-7**, Styrene-divinylbenzene copolymer
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)

RN 9003-70-7 HCA

CN Benzene, diethenyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 1321-74-0
CMF C10 H10
CCI IDS



$2 \left[\text{D1}-\text{CH}{=}\text{CH}_2 \right]$

CM 2

CRN 100-42-5
CMF C8 H8

$H_2C{=}CH-Ph$

IT **7553-56-2**, **Iodine**, uses
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

$I-I$

IT **1333-74-0P**, Hydrogen, processes
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-isotope exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 71-11 (Nuclear Technology)
Section cross-reference(s): 67
IT Isotope separation
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-isotope exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
IT Radioactive wastes
(wastewaters, deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
IT 7440-06-4, Platinum, uses
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
IT **9003-70-7**, Styrene-divinylbenzene copolymer
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
IT **7553-56-2**, **Iodine**, uses
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)
IT 7782-39-0, Deuterium, processes
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-isotope exchange reaction destined for deuterium simulant removal from wastewaters contg. **iodine** in reprocessing plant)
IT **1333-74-0P**, Hydrogen, processes 13670-17-2P, Water-t
(deactivation of hydrophobic Pt/SDBC-catalyst for H2/HTO-isotope exchange reaction destined for tritium removal from wastewaters contg. **iodine** in reprocessing plant)

L58 ANSWER 5 OF 22 HCA COPYRIGHT 2006 ACS on STN
120:163235 Low-Temperature Decomposition of Alkyl Iodides on Ni(100) Surfaces: Evidence for the Formation of Alkyl Free Radicals. Zaera, Francisco; Tjandra, Sariwan (Department of Chemistry, University of California, Riverside, CA, 92521, USA). Journal of Physical Chemistry, 98(11), 3044-9 (English) **1994**. CODEN: JPCHAX. ISSN: 0022-3654.

AB Previous studies have shown that alkyl iodides dissoc. on metal substrates around 200 K to produce **iodine** atoms and alkyl moieties on the surface; here the authors report a new low-temp. decompn. pathway for those compds. on Ni(100) that leads to the formation of a close to 1:1 alkane-alkene mixt. below 150 K. This latter reaction is proposed to occur via a mechanism where alkyl iodide dissocn. results in the direct formation of free radicals. A combination of thermal desorption expts. with isotope labeling and hydrogen coadsorption was used to establish the importance of the nickel surface in the overall process and to rule out either surface disproportionation or gas-phase reactions as the source of the low-temp. products. Evidence was also obtained for a possible rearrangement of the adsorbed alkyl iodide mols. from a flat geometry into an upright configuration at high coverages, a change that would explain the ease with which the radicals formed after C-I bond scission are released into the gas phase instead of being left on the surface as adsorbed alkyl surface moieties. A comparison with other systems is also presented.

IT **74-82-8P**, Methane, preparation **74-98-6P**, Propane, preparation **106-97-8P**, Butane, preparation **109-66-0P**, Pentane, preparation **115-07-1P**, Propene, preparation **1333-74-0P**, **Hydrogen**, **preparation** **25167-67-3P**, Butene **25377-72-4P**, Pentene
(**prepn.**; low-temp. decompn. of alkyl iodides on nickel surfaces: evidence for gas-phase free radical intermediates in formation of alkanes and alkenes)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

$H-H$

RN 25167-67-3 HCA
CN Butene (8CI, 9CI) (CA INDEX NAME)

CM 1

CRN 106-97-8
CMF C4 H10

$H_3C-CH_2-CH_2-CH_3$

RN 25377-72-4 HCA
CN Pentene (8CI, 9CI) (CA INDEX NAME)

CM 1

CRN 109-66-0
CMF C5 H12

$H_3C-CH_2-CH_2-CH_2-CH_3$

CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): 67
IT **74-82-8P**, Methane, preparation **74-98-6P**, Propane, preparation **106-97-8P**, Butane, preparation **109-66-0P**, Pentane, preparation **115-07-1P**, Propene, preparation **1333-74-0P**, **Hydrogen, preparation** **25167-67-3P**, Butene **25377-72-4P**, Pentene
(**prepn.**; low-temp. decompn. of alkyl iodides on nickel surfaces: evidence for gas-phase free radical intermediates in formation of alkanes and alkenes)

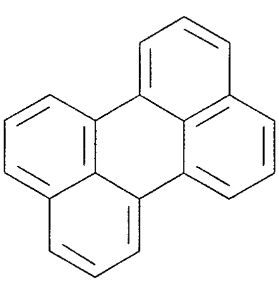
L58 ANSWER 6 OF 22 HCA COPYRIGHT 2006 ACS on STN
110:201412 Fermi level pinning of semiconductor electrodes in aqueous and non aqueous electrolytes: influence of the modification of the electrode surface. Savadogo, O. (Dep. Genie Metall., Ec. Polytech. Montreal, Montreal, QC, H3C 3A7, Can.). Canadian Journal of Chemistry, 67(3), 382-8 (English) **1989.** CODEN: CJCHAG. ISSN: 0008-4042.

AB Modification of several semiconductors material surfaces with H4SiW12O40.nH2O was carried out to produce an increase in the open-circuit photopotential at the semiconductor/electrolyte interface (Voc) without changing the flatband potential. The augmentation of Voc is shown to be attributed to a decrease of the minority carriers recombination at the semiconductor/electrolyte interface along with the suppression of Fermi level pinning. The enhancement of Voc and the electrocatalytic activity of the H evolution reaction in acidic medium of the derivatized electrodes is attributed to the Fermi level unpinning.

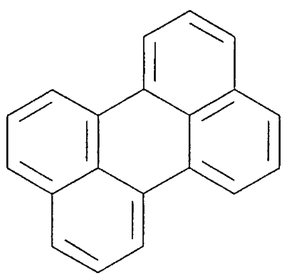
IT **7553-56-2, Iodine**, uses and miscellaneous
(elec. flatband potential of semiconductor electrodes modified with redox couple contg., in dichloroethane)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **198-55-0**, Perylene **12576-62-4**, Perylene radical cation
(elec. flatband potential of semiconductor electrodes modified with redox couple contg., in dichloroethane)
RN 198-55-0 HCA
CN Perylene (8CI, 9CI) (CA INDEX NAME)



RN 12576-62-4 HCA
CN Perylene, radical ion(1+) (9CI) (CA INDEX NAME)



IT **1333-74-0P, Hydrogen, preparation**
(evolution of, photoelectrochem., on semiconductor electrodes modified with tungstosilicic acid)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 72-2 (Electrochemistry)
Section cross-reference(s): 65, 67, 76
IT **7553-56-2, Iodine,** uses and miscellaneous
20461-54-5, Iodide, uses and miscellaneous
(elec. flatband potential of semiconductor electrodes modified with redox couple contg., in dichloroethane)
IT 102-54-5, Ferrocene **198-55-0**, Perylene 12125-80-3, Ferrocenium **12576-62-4**, Perylene radical cation
(elec. flatband potential of semiconductor electrodes modified with redox couple contg., in dichloroethane)
IT **1333-74-0P, Hydrogen, preparation**
(evolution of, photoelectrochem., on semiconductor electrodes modified with tungstosilicic acid)

L58 ANSWER 7 OF 22 HCA COPYRIGHT 2006 ACS on STN
110:181318 Requirements regarding waste containers for permanent disposal. Warnecke, E.; Brennecke, P.; Wurtinger, W.; Gruendler, D. (Phys. Tech. Bundesanst., Braunschweig, 3300, Fed. Rep. Ger.). Ber. Kernforschungsanlage Juelich [Conf.], Juel-Conf-65, Entsorgung Radioakt. Abfaelle, 119-46 (German) **1988.** CODEN: BKJCAW. ISSN: 0366-0885.
AB A safety anal. of the overall geol. and hydrogeol. situation and tech. aspects of the repository and its planned operation and the waste packages provided for terminal storage and discussed for the Konrad repository of the Phys.-Tech. Institute. The derivation of the repository conditions, esp. for the Konrad mine shaft, quantification of the basic requirements, key radionuclide activities, combustibility of the waste, strength and purity of the

materials, free-moving liqs., and gas formation are described. Primary concerns are the operation of the facility, accident response, thermal interfluence of the host rock, criticality safety, and long-term radiol. effects. Several examples are given for the fundamental and group-specific requirements on the waste products.

IT **74-82-8P**, Methane, preparation **1333-74-0P**, **Hydrogen**, **preparation**
(**formation** of, in permanent disposal of radioactive wastes)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 71-11 (Nuclear Technology)

IT **74-82-8P**, Methane, preparation 124-38-9P, Carbon dioxide, preparation **1333-74-0P**, **Hydrogen**, **preparation**
(**formation** of, in permanent disposal of radioactive wastes)

IT 10045-97-3, Cesium-137, uses and miscellaneous 10098-97-2, Strontium-90, uses and miscellaneous 10198-40-0, Cobalt-60, uses and miscellaneous 13966-31-9, Manganese-54, uses and miscellaneous 13981-37-8, Nickel-63, uses and miscellaneous 14681-59-5, Iron-55, uses and miscellaneous 14762-75-5, Carbon-14, uses and miscellaneous 15046-84-1, **Iodine**-129, uses and miscellaneous 15117-48-3, Plutonium-239, uses and miscellaneous
(permanent disposal of radioactive waste contg., containers for)

L58 ANSWER 8 OF 22 HCA

107:187025 Radiolysis of epichlorohydrin in the presence of disperse oxides. Doroshenko, V. N.; Kulish, L. F.; Meleshevich, A. P. (Inst. Fiz. Khim., Kiev, USSR). Ukrainskii Khimicheskii Zhurnal (Russian Edition), 53(6), 596-9 (Russian) **1987.** CODEN: UKZHAU. ISSN: 0041-6045.

AB Compn. of the radiolysis products in the mixts. of epichlorohydrin (I) and oxides (SiO_2, Al_2O_3), in monolayers of I adsorbed on oxides, or for **pure I** was the same and comprises H, CO, CH_4, C_2H_4, and C_2H_2. At the oxide concn. (c) .ltoreq.40 wt.% concn. of the **products** vary little (**H**, C_2H_4) or did not depend (Co, CH_4, C_2H_2) on c. Increase of the radiolysis degree of I

was obsd. at c >70 wt.% or <30 effective monolayers of I. For 1-5 monolayers of I on SiO2 or Al2O3 the C2H4 and C2H2 products were not obsd. In a monolayer of I on SiO2 concn. of CO increased 7 times, in 4 monolayers of I on Al2O3 4 times, compared to that in homogeneous I. Formation of CO and CH4 in polylayers had antibate character.

IT **74-82-8P**, Methane, preparation **74-85-1P**, Ethylene, preparation **74-86-2P**, Acetylene, preparation **1333-74-0P, Hydrogen, preparation**
(**formation** of, in radiolysis of epichlorohydrin adsorbed or in mixts. with silica gel or aluminum oxide)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 74-86-2 HCA
CN Ethyne (9CI) (CA INDEX NAME)

$HC{\equiv}CH$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

$H{-}H$

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **74-82-8P**, Methane, preparation **74-85-1P**, Ethylene, preparation **74-86-2P**, Acetylene, preparation 630-08-0P, Carbon monoxide, preparation **1333-74-0P**, **Hydrogen, preparation**
(**formation** of, in radiolysis of epichlorohydrin adsorbed or in mixts. with silica gel or aluminum oxide)

L58 ANSWER 9 OF 22 HCA COPYRIGHT 2006 ACS on STN

104:58400 Investigations on the reduction of methanol for the development of the hydrocarbon hybrid cycle. Biallas, B.; Weirich, W.; Kuegler, B.; Oertel, M.; Pietsch, M.; Winkelmann, U. (Univ.

Aachen, Aachen, Fed. Rep. Ger.). International Journal of Hydrogen Energy, 10(10), 661-5 (English) **1985**. CODEN: IJHEDX.
ISSN: 0360-3199.

AB The hydrocarbon hybrid cycle requires a step to reduce CH3OH. A sequence of reactions was investigated using I to reduce the cell voltage and formation of CH3I as an intermediate compd. Electrolytic expts. show that a cell voltage of 1 V at 1 kA m-2 can be obtained. Methane resulted from the gas-phase reaction of CH3I and H2O. A mass flow balance was set up to generate a closed cycle, considering operating conditions which are suitable for a steam reformer and a MeOH synthesis reactor.

IT **7553-56-2**, uses and miscellaneous
(cathodic depolarizer, for methane prodn. from methanol with Me iodide intermediate)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

IT **1333-74-0P**, preparation
(evolution of, in hydrocarbon hybrid cycle with electrochem. formation of methyliodide)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H— H

IT **74-82-8P**, preparation
(formation of, by gas-phase reaction of methyliodide and water in hydrocarbon hybrid cycle, **iodine** cathodic depolarizer in relation to)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

CC 72-9 (Electrochemistry)
Section cross-reference(s): 23, 49

ST methanol redn hydrocarbon hybrid cycle; **iodine** cathodic depolarizer methanol redn; methane prodn methanol **iodine** depolarizer; potential methane prodn methanoliodine; water electrolysis hydrocarbon hybrid cycle

IT Electrolytic depolarizers
(cathodic, **iodine**, for methane prodn. from methanol with Me iodide intermediate)

IT Hydrolysis
 (of methyliodide in methane prodn. in hydrocarbon hybrid cycle, **iodine** cathodic depolarizer in)
IT **7553-56-2**, uses and miscellaneous
 (cathodic depolarizer, for methane prodn. from methanol with Me iodide intermediate)
IT 7732-18-5, uses and miscellaneous
 (electrolysis of, hydrocarbon hybrid cycle with **iodine** cathodic depolarizer in relation to)
IT **1333-74-0P**, preparation 7782-44-7P, preparation
 (evolution of, in hydrocarbon hybrid cycle with electrochem. formation of methyliodide)
IT **74-82-8P**, preparation
 (formation of, by gas-phase reaction of methyliodide and water in hydrocarbon hybrid cycle, **iodine** cathodic depolarizer in relation to)
IT 74-88-4P, preparation
 (formation of, electrochem., **iodine** cathodic depolarizer in, in methane prodn. in hydrocarbon hybrid cycle)
IT 67-56-1, reactions
 (redn. of, hydrocarbon hybrid cycle in, **iodine** cathodic depolarizer in relation to)

L58 ANSWER 10 OF 22 HCA
100:182073 Catalyst for hydrogen isotope exchange. (Agency of Industrial Sciences and Technology, Japan; Hikari Kogyo Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 58177152 A2 **19831017** Showa, 8 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1982-60336 19820413.
AB A catalyst-bearing structure useful in heavy water **prodn.** via **H**-water isotope exchange and in removing I from water was obtained by filling the voids in a net prepd. with a hydrophilic fiber with a H exchange catalyst supported on a hydrophobic material.
IT **9002-88-4**
 (in porous network for catalysts for hydrogen isotope exchange reaction for heavy water prodn.)
RN 9002-88-4 HCA
CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1
CMF C2 H4

$H_2C{=}CH_2$

IT **7553-56-2**, uses and miscellaneous

(removal of, from water, catalyst of porous network filled with platinum for)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

IT **1333-74-0DP**, isotopes, preparation
(sepn. of, catalysts for)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IC B01J035-06; B01J031-28
ICA B01D059-32; C01B005-02
CC 71-6 (Nuclear Technology)
Section cross-reference(s): 67
IT Polyamide fibers, uses and miscellaneous
Synthetic fibers
(hydrophilic, in catalysts net **prepn.** for **hydrogen** isotope exchange)
IT 9002-84-0 **9002-88-4**
(in porous network for catalysts for hydrogen isotope exchange reaction for heavy water prodn.)
IT **7553-56-2**, uses and miscellaneous
(removal of, from water, catalyst of porous network filled with platinum for)
IT **1333-74-0DP**, isotopes, preparation
(sepn. of, catalysts for)

L58 ANSWER 11 OF 22 HCA
97:171289 The methane-methanol hybrid cycle. Biallas, B.; Behr, F.; Hunsaenger, K.; Kuegler, B.; Weirich, W.. (Aachen, D-5100, Fed. Rep. Ger.). Advances in Hydrogen Energy, 3(Hydrogen Energy Prog. 4, Vol. 2), 579-90 (English) **1982.** CODEN: AHENDB. ISSN: 0276-2412.
AB The CH4-CH3OH hybrid cycle for the **prodn.** of **H** from H2O consists of 3 steps: (1) a steam reformer, heated by a high temp. nuclear reactor, (2) MeOH synthesis, and (3) the redn. of MeOH by electrolysis. Since the redn. of MeOH at potentials lower than that of H evolution is not yet known, it remains the only step still to be taken in the development of a complete **H producing** plant as presented here. Calcns. are based on a high temp. reactor whose thermal power is 500 MW. The result is a **H producing** rate of 1991 kmol/h. The expts.

carried out on the key reaction show the desired depolarization of the cathode by means of I and the formation of CH4 using addnl. catalysts.

IT **74-82-8**, uses and miscellaneous
(-methanol hybrid cycle)
RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

IT **7553-56-2**, uses and miscellaneous
(electrolytic depolarizer, methane-methanol hybrid cycle for **hydrogen prodn.** in relation to)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

IT **1333-74-0P**, preparation
(manuf. of, from water, methane-methanol cycle in relation to)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H— H

CC 72-9 (Electrochemistry)
Section cross-reference(s): 52
ST methane methanol hybrid cycle hydrogen; redn electrochem methanol **hydrogen prodn**; water methane thermal reaction hydrogen
IT Electrolytic depolarizers
(**iodine**, methane-methanol hybrid cycle for **hydrogen prodn.** in relation to)
IT Reduction, electrochemical
(of methanol, methane-methanol hybrid cycle for **hydrogen prodn.** in relation to)
IT **74-82-8**, uses and miscellaneous
(-methanol hybrid cycle)
IT **7553-56-2**, uses and miscellaneous
(electrolytic depolarizer, methane-methanol hybrid cycle for **hydrogen prodn.** in relation to)
IT 7732-18-5, uses and miscellaneous
(**hydrogen prodn.** from, methane-methanol hybrid cycle in relation to)
IT **1333-74-0P**, preparation

(manuf. of, from water, methane-methanol cycle in relation to)

L58 ANSWER 12 OF 22 HCA

97:82582 Gas-phase radiolysis of trifluoromethyl iodide/methyl iodide mixtures. Teclemariam, Dawit; Hanrahan, Robert J. (Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA). Radiation Physics and Chemistry, 19(6), 443-8 (English) **1982.** CODEN: RPCHDM. ISSN: 0146-5724.

AB The gas phase radiolysis of equimolar mixts. of MeI and CF3I was studied at 200 torr (26.7 kPa) pressure both pure and with 10% added O. For the pure system 21 products were identified and their yields measured. The major products and their G-values are: HI 1.56, HF 1.04, **I2** 0.76, H2 0.42, CH4 0.35, C2H6 0.25, CF3H 0.34, CH2I2 3.08, and C2F4I2 0.26. Minor products include CF4, C2F6, C2F4, C2H4, C2H2, C2H2F2, CH3CF3, C2F3H, C2F2HI, C2F3I, C2F5I and C2H2F3I. The addn. of 10% O reduced the products significantly except that the C2H4, CHF3 and **I2** yields were enhanced. Although ionic pathways contribute to formation of some products, rupture of the weak C-I bond in both reactants is of major importance in this system. Attack of the resulting CF3- and CH3- radicals on substrate (esp. CH3I) via abstraction and displacement reactions accounts for most of the major product yields. The overall yield for decompn. of CH3I during radiolysis of the mixts. exceeds the yield for decompn. of CF3I by a factor of nearly three.

IT **74-82-8P**, preparation **74-84-0P**, preparation
74-85-1P, preparation **74-86-2P**, preparation
1333-74-0P, preparation **7553-56-2P**, preparation
(formation of, in radiolysis of trifluoromethyl iodide-Me iodide mixts., mechanism of)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

RN 74-86-2 HCA

CN Ethyne (9CI) (CA INDEX NAME)

HC≡CH

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **74-82-8P**, preparation **74-84-0P**, preparation
74-85-1P, preparation **74-86-2P**, preparation
75-11-6P 75-46-7P 75-73-0P 76-16-4P 116-14-3P, preparation
353-83-3P 354-64-3P 354-65-4P 359-11-5P 359-37-5P
420-46-2P 1320-41-8P **1333-74-0P**, preparation
2925-16-8P **7553-56-2P**, preparation 7664-39-3P,
preparation 10034-85-2P
(formation of, in radiolysis of trifluoromethyl iodide-Me iodide mixts., mechanism of)

L58 ANSWER 13 OF 22 HCA COPYRIGHT 2006 ACS on STN
93:157325 **Production** of fast **hydrogen** atoms by stripping hydride ions in gas and vapor targets. Anderson, C. J.; Girnius, R. J.; Howald, A. M.; Anderson, L. W. (Dep. Phys., Univ. Wisconsin, Madison, WI, 53706, USA). Physical Review A: Atomic, Molecular, and Optical Physics, 22(3), 822-34 (English) **1980**
. CODEN: PLRAAN. ISSN: 0556-2791.
AB Measurements of the total charge-changing cross sections to strip 1 and 2 e from a H- ion are reported for 30-200-keV H-ions incident on Ne, Ar, Kr, Xe, Li, Na, K, Rb, and Cs gas or vapor targets. Measurements of the total charge-changing cross sections to strip an e from a fast ground-state H0 atom and to **form** a **H** - ion from a fast ground-state H0 atom are reported for 30-200-keV fast ground-state H0 atoms incident on the same targets. Measurements are also reported on the fractional yields as a function of the target thickness for 30-200-keV H- ions incident on a variety of targets. The neutral fraction increases, reaches a max. value, F0max, and then decreases to the equil. fraction F0.infin. as the target thickness increases from 0 to a very large

value. Measurements of F0max, F0.infin., and F.infin. are reported for H- ions incident on a variety of targets.

IT **106-97-8P**, uses and miscellaneous **109-66-0P**, uses and miscellaneous **1333-74-0P**, uses and miscellaneous **7553-56-2P**, uses and miscellaneous
(targets, fast **hydrogen** atom **prodn.** by stripping hydride ions in)

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-CH_3$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 71-1 (Nuclear Technology)
ST fusion **hydrogen** atom **prodn** stripping; hydride stripping hydrogen atom fusion; cross section electron stripping hydride
IT Nuclear targets
(hydride ion stripping in gas and vapor, fast **hydrogen** atom **prodn.** from)
IT Nuclear fusion
(**hydrogen** atom **prodn.** by collisional stripping of hydride ions in relation to)
IT Natural gas
(targets, fast **hydrogen** atom **prodn.** by stripping hydride ions in)
IT 67-64-1P, uses and miscellaneous 75-46-7P 75-63-8P 75-73-0P **106-97-8P**, uses and miscellaneous **109-66-0P**, uses and miscellaneous 124-38-9P, uses and miscellaneous **1333-74-0P**, uses and miscellaneous 2551-62-4P

7439-90-9P, uses and miscellaneous 7439-93-2P, uses and miscellaneous 7440-01-9P, uses and miscellaneous 7440-09-7P, uses and miscellaneous 7440-17-7P, uses and miscellaneous 7440-23-5P, uses and miscellaneous 7440-37-1P, uses and miscellaneous 7440-46-2P, uses and miscellaneous 7440-59-7P, uses and miscellaneous 7440-63-3P, uses and miscellaneous **7553-56-2P**, uses and miscellaneous 7726-95-6P, uses and miscellaneous 7727-37-9P, uses and miscellaneous 7732-18-5P, uses and miscellaneous 7782-39-0P, uses and miscellaneous 7782-44-7P, uses and miscellaneous
(targets, fast **hydrogen** atom **prodn.** by stripping hydride ions in)

L58 ANSWER 14 OF 22 HCA COPYRIGHT 2006 ACS on STN
92:114962 Material corrosion investigations for the General Atomic sulfur-**iodine** thermochemical water-splitting cycle.
Trester, P. W.; Liang, S. S. (Gen. At. Co., San Diego, CA, USA). Advances in Hydrogen Energy, 1(Hydrogen Energy Syst., Vol. 4), 2113-59 (English) **1979.** CODEN: AHENDB. ISSN: 0276-2412.

AB Corrosion resistance of candidate construction materials for conducting the S-I cycle in the **prodn.** of **H** was investigated in anticipated process fluids. Coated and uncoated Incoloy 800H [60616-02-6], AISI 304 [11109-50-5] stainless steel, and Inconel 600 [12606-02-9] alloys were exposed .ltoreq.1000 h in the vapor of decompg. H2SO4 at 1173 K. The uncoated alloys sustained grain boundary attack, but aluminized Incolay 800H was resistant. In aq. solns. contg. HI and I at 295-407 K, Durichlor 51 [39467-36-2] and Chlorimet 2 [12605-66-2] alloys resisted rapid dissoln. after a few weeks exposure. Zr, Ta, Nb, and Mo were corrosion-resistant under boiling conditions, and Ti was attacked after 100 h. A perfluorocarbon elastomer, borosilicate glass, graphite, and several fluorocarbon plastics were resistant to HIx.

IT **9010-79-1D**, fluorinated
(corrosion resistance of, in aq. soln. contg. hydriodic acid and **iodine**)

RN 9010-79-1 HCA

CN 1-Propene, polymer with ethene (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1
CMF C3 H6

$H_3C-CH=CH_2$

CM 2

CRN 74-85-1
CMF C2 H4

$H_2C{=}CH_2$

IT **1333-74-0P**, properties
(prepn. of, by sulfur-**iodine** cycle, corrosion resistance of materials for)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

CC 56-8 (Nonferrous Metals and Alloys)
Section cross-reference(s): 49
ST **hydrogen prodn** alloy corrosion; stainless steel corrosion **hydrogen prodn**; nickel alloy corrosion **hydrogen prodn**; iron alloy corrosion **hydrogen prodn**; perfluorocarbon elastomer corrosion **hydrogen prodn**; fluorocarbon plastic corrosion **hydrogen prodn**; graphite corrosion **hydrogen prodn**; glass corrosion **hydrogen prodn**
IT Glass, oxide
(borosilicate, corrosion resistance of, in aq. soln. contg. hydriodic acid and **iodine**)
IT Corrosion
(resistance to, of materials for **hydrogen prodn** . by sulfur-**iodine** thermochem. water-splitting cycle)
IT Rubber, synthetic
(tetrafluoroethylene-trifluoromethyl trifluorovinyl ether, corrosion resistance of, in aq. soln. contg. hydriodic acid and **iodine**)
IT 7439-98-7, properties 7440-03-1, properties 7440-25-7, properties 7440-32-6, properties 7440-67-7, properties 7782-42-5, properties 9002-83-9 **9010-79-1D**, fluorinated 12605-66-2 39467-36-2 72980-82-6
(corrosion resistance of, in aq. soln. contg. hydriodic acid and **iodine**)
IT **1333-74-0P**, properties
(prepn. of, by sulfur-**iodine** cycle, corrosion resistance of materials for)

L58 ANSWER 15 OF 22 HCA COPYRIGHT 2006 ACS on STN
92:13588 Radiolytic decomposition of tetraethylammonium iodide in solid

state. I. The main stable products. Sofronie, E. (Inst. Nucl. Phys. Eng., Bucharest, Rom.). Radiochemical and Radioanalytical Letters, 40(2), 79-86 (English) **1979.** CODEN: RRALAZ. ISSN: 0079-9483.

AB The .gamma.-radiolysis of Et4NI in the solid state gives as main stable **products**: **H2**, C1-4 hydrocarbons, **I2**, and a solid residue. Radiolytic yields of all products decrease on increasing either the dose rate or the integral dose.

IT **74-84-0P**, preparation **74-85-1P**, preparation **1333-74-0P**, preparation **2465-56-7P** **7553-56-2P**, preparation
(formation of, in radiolysis of tetraethylammonium iodide in solid phase)

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

RN 2465-56-7 HCA
CN Methylene (8CI, 9CI) (CA INDEX NAME)

CH_2

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)

IT **74-84-0P**, preparation **74-85-1P**, preparation
74-88-4P, preparation 75-03-6P 75-04-7P, preparation
109-89-7P, preparation 121-44-8P, preparation **1333-74-0P**

, preparation **2465-56-7P** **7553-56-2P**, preparation
(formation of, in radiolysis of tetraethylammonium iodide in solid phase)

L58 ANSWER 16 OF 22 HCA COPYRIGHT 2006 ACS on STN
83:170789 The .gamma.-radiolysis of 3-iodopropanoic acid. Borghi, Elena; Quintiliani, Marcello (Lab. Chim. Biol., Ist. Super. Sanita, Rome, Italy). Annali di Chimica (Rome, Italy), 64(5-6), 265-74 (Italian) **1974.** CODEN: ANCRAI. ISSN: 0003-4592.

AB Preliminary qual. results on the radiolysis of 10-2M aqueous solns. of 3-iodopropanoic acid (IPA) under 60Co .gamma.-rays are reported. The compn. of the samples (both aqueous and gaseous phase) after irradn. at various doses was qual. detd. by spectrophotometric and gas-chromatog. methods. Adipic acid was obsd. in the aq. phase. CH4, C2H6, C2H4, H2, CO, CO2, I, propylene, 1-butene, butane, CH3I, EtI and .beta.-propanoic acid lactone were obsd. in the gaseous phase. The G(-IPA) value for samples irradiated under an Ar atm. was 5.2. A linear relation was obsd. between IPA decompn. and received dose up to 40% disappearance. Some reactions are suggested to explain the observed decompn. products.

IT **74-82-8P**, preparation **74-84-0P**, preparation
74-85-1P, preparation **106-97-8P**, preparation
106-98-9P, preparation **115-07-1P**, preparation
1333-74-0P, preparation **7553-56-2P**, preparation
(formation of, in radiolysis of iodopropanoic acid in aq. soln.)

RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C{=}CH_2$

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 106-98-9 HCA
CN 1-Butene (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH=CH_2$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I-I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 57-57-8P **74-82-8P**, preparation **74-84-0P**, preparation **74-85-1P**, preparation 74-88-4P 75-03-6P **106-97-8P**, preparation **106-98-9P**, preparation **115-07-1P**, preparation 124-04-9P, preparation 124-38-9P, preparation 630-08-0P, preparation **1333-74-0P**, preparation **7553-56-2P**, preparation
(formation of, in radiolysis of iodopropanoic acid in aq. soln.)

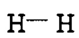
L58 ANSWER 17 OF 22 HCA COPYRIGHT 2006 ACS on STN
81:8332 Yields of elementary reactions initiated when hydrogen iodide and deuterium iodide are activated by 254 nm radiation in 3-methylpentane-h14 and -d14 at 20-300.deg.K. Hydrogen atom trapping. Perkey, Lewis; Willard, John E. (Dep. Chem., Univ. Wisconsin, Madison, WI, USA). Journal of Chemical Physics, 60(7), 2732-40 (English) **1974.** CODEN: JCPSA6. ISSN: 0021-9606.
AB The photolysis of HI or DI in 3-methylpentane (I) or perdeuterated-I at 77.degree.K using Hg arc lamp radiation and the resulting ESR spectra show that the matrix isotope effect, i.e. trapped **H** atoms are **formed** in 254-nm photolyzed HI in perdeuterated-I at <50.degree.K and not in HI-I glass, is probably due to the absence of thermal H atoms. Quantum yields are given for

trapped radicals, alkyl iodides, and **I2** produced at
77.degree.K, and literature values for **H prodn.**
from 300-77.degree.K are reevaluated to better understand the
photoreactions of HI in matrixes.

IT **1333-74-0P**, preparation **7553-56-2P**, preparation
(formation of, in photolysis of hydrogen iodide in methylpentane glass)

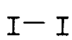
RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)



RN 7553-56-2 HCA

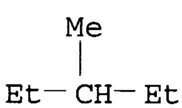
CN Iodine (8CI, 9CI) (CA INDEX NAME)



IT **96-14-0 20586-83-8**
(photolysis of hydrogen iodide in, matrix isotope effect of)

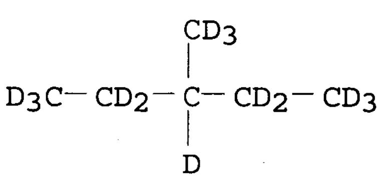
RN 96-14-0 HCA

CN Pentane, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 20586-83-8 HCA

CN Pentane-1,1,1,2,2,3,4,4,5,5,5-d11, 3-(methyl-d3)- (9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
Section cross-reference(s): 73

IT **1333-74-0P**, preparation **7553-56-2P**, preparation
(formation of, in photolysis of hydrogen iodide in methylpentane glass)

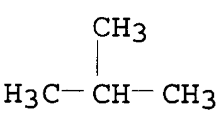
IT **96-14-0 20586-83-8**
(photolysis of hydrogen iodide in, matrix isotope effect of)

L58 ANSWER 18 OF 22 HCA COPYRIGHT 2006 ACS on STN
80:139428 Gamma radiolysis of branched chain hydrocarbons. 2,3-Dimethylbutane. Castello, Gianrico; Grandi, Francesco; Munari, Stelio (Ist. Chim. Ind., Univ. Genova, Genoa, Italy). Radiation Research, 58(2), 176-89 (English) **1974.** CODEN: RAREAE. ISSN: 0033-7587.

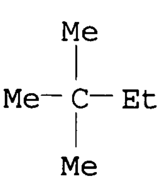
AB The .gamma.-radiolysis of liq. 2,3-dimethylbutane at room temp. was investigated under vacuum. **Iodine** was used as a free radical scavenger and the formed alkyl iodides were analyzed by gas chromatog. with electron capture detector. Irradns. of frozen 2,3-dimethylbutane at 77.degree.K were also performed. The fragmentation products and many of those having a no. of C atoms higher than the parent were identified and measured. The formation of the identified heavy products is mainly due to recombination of radicals, as demonstrated by the comparison between their yields and those of alkyl iodides.

IT **75-28-5P 75-83-2P 78-78-4P**
78-79-5P, preparation **115-11-7P**, preparation
464-06-2P 513-35-9P 563-45-1P
563-46-2P 563-78-0P 563-79-1P
565-59-3P 1069-53-0P 3074-71-3P
16747-28-7P 16747-38-9P 52670-32-3P
52670-33-4P 52670-34-5P 52670-35-6P
52670-36-7P
(formation of, in radiolysis of dimethylbutane in presence of **iodine**)

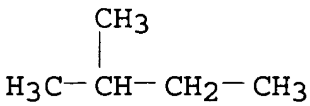
RN 75-28-5 HCA
CN Propane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



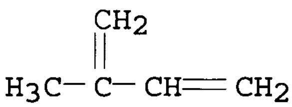
RN 75-83-2 HCA
CN Butane, 2,2-dimethyl- (8CI, 9CI) (CA INDEX NAME)



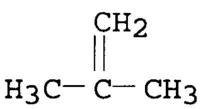
RN 78-78-4 HCA
CN Butane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



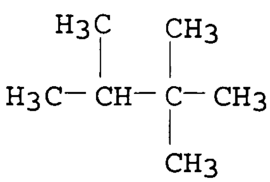
RN 78-79-5 HCA
CN 1,3-Butadiene, 2-methyl- (9CI) (CA INDEX NAME)



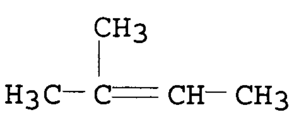
RN 115-11-7 HCA
CN 1-Propene, 2-methyl- (9CI) (CA INDEX NAME)



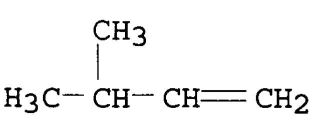
RN 464-06-2 HCA
CN Butane, 2,2,3-trimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 513-35-9 HCA
CN 2-Butene, 2-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

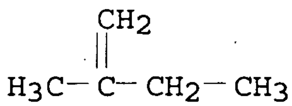


RN 563-45-1 HCA
CN 1-Butene, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

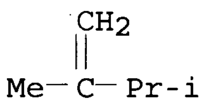


RN 563-46-2 HCA

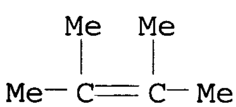
CN 1-Butene, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



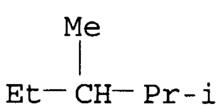
RN 563-78-0 HCA
CN 1-Butene, 2,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



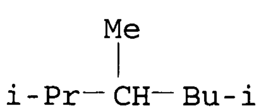
RN 563-79-1 HCA
CN 2-Butene, 2,3-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



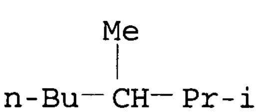
RN 565-59-3 HCA
CN Pentane, 2,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 1069-53-0 HCA
CN Hexane, 2,3,5-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

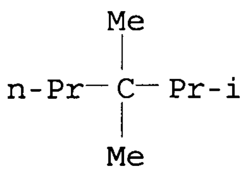


RN 3074-71-3 HCA
CN Heptane, 2,3-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

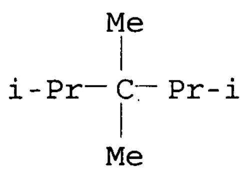


RN 16747-28-7 HCA

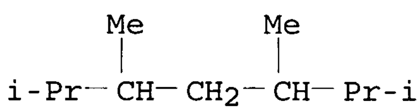
CN Hexane, 2,3,3-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



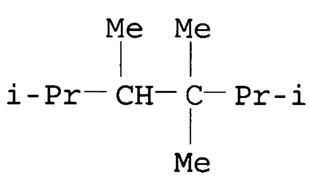
RN 16747-38-9 HCA
CN Pentane, 2,3,3,4-tetramethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



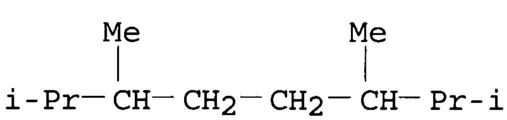
RN 52670-32-3 HCA
CN Heptane, 2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)



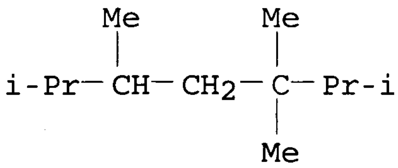
RN 52670-33-4 HCA
CN Hexane, 2,3,3,4,5-pentamethyl- (9CI) (CA INDEX NAME)



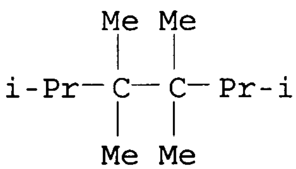
RN 52670-34-5 HCA
CN Octane, 2,3,6,7-tetramethyl- (9CI) (CA INDEX NAME)



RN 52670-35-6 HCA
CN Heptane, 2,3,3,5,6-pentamethyl- (9CI) (CA INDEX NAME)



RN 52670-36-7 HCA
CN Hexane, 2,3,3,4,4,5-hexamethyl- (9CI) (CA INDEX NAME)



IT **74-82-8P**, preparation **74-84-0P**, preparation
74-85-1P, preparation **74-86-2P**, preparation
74-98-6P, preparation **106-97-8P**, preparation
106-98-9P, preparation **106-99-0P**, preparation
115-07-1P, preparation **590-18-1P** **624-64-6P**
1333-74-0P, preparation
(formation of, in radiolysis of dimethylbutane, dose and **iodine** effect on)
RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

RN 74-86-2 HCA
CN Ethyne (9CI) (CA INDEX NAME)

$HC\equiv CH$

RN 74-98-6 HCA
CN Propane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_3$

RN 106-97-8 HCA
CN Butane (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_3$

RN 106-98-9 HCA
CN 1-Butene (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH_2-CH=CH_2$

RN 106-99-0 HCA
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

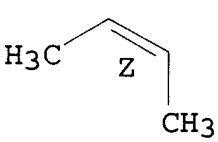
$H_2C=CH-CH=CH_2$

RN 115-07-1 HCA
CN 1-Propene (9CI) (CA INDEX NAME)

$H_3C-CH=CH_2$

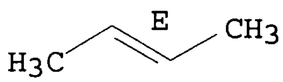
RN 590-18-1 HCA
CN 2-Butene, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 624-64-6 HCA
CN 2-Butene, (2E)- (9CI) (CA INDEX NAME)

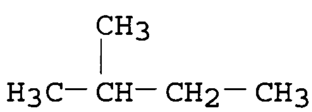
Double bond geometry as shown.



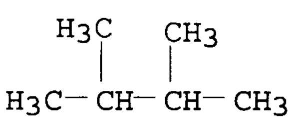
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **78-78-4P**
(prepn. of)
RN 78-78-4 HCA
CN Butane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



IT **79-29-8**
(radiolysis of liq. and frozen, radical reactions in)
RN 79-29-8 HCA
CN Butane, 2,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



IT **7553-56-2**, uses and miscellaneous
(scavenger, of free radicals in radiolysis of dimethylbutane)
RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
ST dimethylbutane radiolysis; **iodine** radical scavenger dimethylbutane; butane dimethyl radiolysis
IT Radicals, preparation
(formation of, in radiolysis of dimethylbutane in presence of **iodine**)
IT 74-88-4P 75-03-6P **75-28-5P** 75-30-9P **75-83-2P** **78-78-4P** **78-79-5P**, preparation 107-08-4P

115-11-7P, preparation **464-06-2P** **513-35-9P**
513-38-2P 541-28-6P 558-17-8P **563-45-1P**
563-46-2P **563-78-0P** **563-79-1P**
565-59-3P 594-38-7P 594-59-2P 616-14-8P
1069-53-0P **3074-71-3P** **16747-28-7P**
16747-38-9P 18295-27-7P 31295-00-8P **52670-32-3P**
52670-33-4P **52670-34-5P** **52670-35-6P**
52670-36-7P
(formation of, in radiolysis of dimethylbutane in presence of **iodine**)

IT **74-82-8P**, preparation **74-84-0P**, preparation
74-85-1P, preparation **74-86-2P**, preparation
74-98-6P, preparation **106-97-8P**, preparation
106-98-9P, preparation **106-99-0P**, preparation
115-07-1P, preparation **590-18-1P** **624-64-6P**
1333-74-0P, preparation
(formation of, in radiolysis of dimethylbutane, dose and **iodine** effect on)

IT **78-78-4P**
(prepn. of)

IT **79-29-8**
(radiolysis of liq. and frozen, radical reactions in)

IT **7553-56-2**, uses and miscellaneous
(scavenger, of free radicals in radiolysis of dimethylbutane)

L58 ANSWER 19 OF 22 HCA

77:12224 Effect of water on the yields of hydrogen and methane in .gamma.-irradiated C5-hydrocarbons. Bryl-Sandelewska, T. (Dep. Radiat. Chem., Inst. Nucl. Res., Warsaw, Pol.). Radiochemical and Radioanalytical Letters, 9(2), 105-12 (English) **1972.** CODEN: RRALAZ. ISSN: 0079-9483.

AB 60Co .gamma.-irradn. of isopentane (I), n-pentane (II), or cyclopentane (III), mixed 1:1 by vol. with H2O, at a dose rate of 6.2 .times. 1018 eV/ml-hr produced some higher yields of H2 and CH4 than did irradn. of **pure I**, II, or III (compd. irradiated, G(H2), and G(CH4) given: **pure I**, 3.62, 0.70; I with H2O, 3.40, 0.83; pure II, 3.80, 0.20; II with H2O, 4.42, 0.34; pure III, 4.20, 0.045; III with H2O, 3.40, 0.064). A relation was obsd. between increased product yields and the mutual solubilities of I, II, and III with H2O.

IT **74-82-8P**, preparation **1333-74-0P**, preparation
(formation of, in radiolysis of aq. hydrocarbons)

RN 74-82-8 HCA

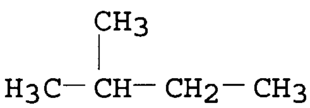
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

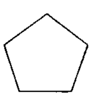
IT **78-78-4 109-66-0 287-92-3**
(radiolysis of aq., hydrogen and methane yields in)
RN 78-78-4 HCA
CN Butane, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 109-66-0 HCA
CN Pentane (8CI, 9CI) (CA INDEX NAME)

$H_3C—CH_2—CH_2—CH_2—CH_3$

RN 287-92-3 HCA
CN Cyclopentane (8CI, 9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **74-82-8P**, preparation **1333-74-0P**, preparation
(formation of, in radiolysis of aq. hydrocarbons)
IT **78-78-4 109-66-0 287-92-3**
(radiolysis of aq., hydrogen and methane yields in)

L58 ANSWER 20 OF 22 HCA COPYRIGHT 2006 ACS on STN
72:84867 Photolysis of ethyl iodide at 77 K. Barker, P. George; Purnell, J. H. (Dep. Chem., Univ. Coll., Swansea, UK). Transactions of the Faraday Society, 66(1), 163-74 (English) **1970.** CODEN: TFSOA4. ISSN: 0014-7672.
AB Detailed anal. studies of the 253.7 nm photolysis of films of pureEtI at 77.degree.K establish that the initial photoprocess leads exclusively to formation of C2H4 and HI with a quantum yield of 0.36. The quantum yield for Et radical formation is estd. as 5 .times. 10-4 from a study of the CF3CH2I photolysis and comparison with earlier work. The formation of C2H6, **I2**, n-C4H10 and

H2 is entirely secondary in nature, and the relative yield are time and Et I-concn. independent. Secondary photolysis involves the complex Et I.HI rather than free HI. A mechanism based on the photolysis of Et I aggregates and cage-formed complexes is proposed, and the marked photoinhibition obsd. as reaction proceeds is established to be a consequence of formation of the further complex, Et I.**I2**.HI, for which a cyclic structure is proposed.

IT **74-84-0P**, preparation **74-85-1P**, preparation
1333-74-0P, preparation **7553-56-2P**, preparation
(formation of, in photolysis of solid iodoethane)

RN 74-84-0 HCA
CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA
CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

RN 7553-56-2 HCA
CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **74-84-0P**, preparation **74-85-1P**, preparation
1333-74-0P, preparation **7553-56-2P**, preparation
10034-85-2P
(formation of, in photolysis of solid iodoethane)

L58 ANSWER 21 OF 22 HCA COPYRIGHT 2006 ACS on STN
69:72778 Gamma-ray-induced radiolysis of propionaldehyde in the liquid phase. Tolgyesi, M.; Marta, F. (Attila Jozsef Univ., Szeged, Hung.). Acta Physica et Chemica, 14(1-2), 27-38 (English) **1968.** CODEN: AUSHAF. ISSN: 0001-6721.
AB Products of the.gamma.-ray induced decompn. of EtCHO and their G-values were detd. as a function of dose intensity, concn., time of irradn., and inhibiting effect of I and NO. Decompn. followed a

chain mechanism involving free radicals, which became more dominant with an increase of dose.

IT **74-84-0P**, preparation **74-85-1P**, preparation **1333-74-0P**, preparation
(formation of, in radiolysis of propionaldehyde)

RN 74-84-0 HCA

CN Ethane (8CI, 9CI) (CA INDEX NAME)

H_3C-CH_3

RN 74-85-1 HCA

CN Ethene (9CI) (CA INDEX NAME)

$H_2C=CH_2$

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H—H

IT **7553-56-2**, uses and miscellaneous
(radiolysis of propionaldehyde in presence of)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I—I

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)

IT 67-64-1P, preparation **74-84-0P**, preparation **74-85-1P**, preparation 78-83-1P 630-08-0P, preparation **1333-74-0P**, preparation
(formation of, in radiolysis of propionaldehyde)

IT **7553-56-2**, uses and miscellaneous 10102-43-9, uses and miscellaneous
(radiolysis of propionaldehyde in presence of)

L58 ANSWER 22 OF 22 HCA

67:59532 Pulse radiolysis of aqueous solutions of alkyl halides. I. Methyl io dide solutions. Thomas, John Kerry (Argonne Natl. Lab., Argonne, IL, USA). Proc. Tihany Symp. Radiat. Chem., 2nd , Meeting Date 1966, 115-22 (English) **1967.** CODEN: 16SOAP.

AB MeI aq. solns. were irradiated by pulses of 15 Mev. electrons. Two stable species were produced: (1) the iodide ion, with a limit of <80 nsec. on the lifetime of any neg. ion intermediate, and (2) an I

atom complex with MeI, [I(CH3I)]. Also produced in small amts. were H, CH3, HI, and CH4. The kinetics demonstrated the feasibility of use of MeI as a source of Me radicals and I atoms in H2O.

IT **7553-56-2P**, preparation
(atomic, formation of, in radiolysis of aq. iodomethane)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

IT **74-82-8P**, preparation **1333-74-0P**, preparation **2229-07-4P**
(formation of, in radiolysis of aq. iodomethane)

RN 74-82-8 HCA

CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H— H

RN 2229-07-4 HCA

CN Methyl (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

CH_3

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)

IT **7553-56-2P**, preparation
(atomic, formation of, in radiolysis of aq. iodomethane)

IT **74-82-8P**, preparation **1333-74-0P**, preparation **2229-07-4P** 10034-85-2P 16812-15-0P 20461-54-5P, preparation
(formation of, in radiolysis of aq. iodomethane)

=> d l59 1-27 ti

L59 ANSWER 1 OF 27 HCA

TI A simple method for the displacement of bromine by fluorine at tertiary, benzylic or non-classical secondary sites

L59 ANSWER 2 OF 27 HCA

TI A simple and versatile method for the hydroiodination of alkenes and alkynes using **I2** and Et3SiH in the presence of copper(II)

L59 ANSWER 3 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Process for preparing of xanthophylls via oxidation of carotenoids

L59 ANSWER 4 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Reactor and **production** of **hydrogen** iodide using same.

L59 ANSWER 5 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Conversion of methane for higher hydrocarbon fuel synthesis using pulsed discharge plasma method

L59 ANSWER 6 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Bond Rupture in the Radiolysis of n-Alkanes: An Application of Gel Permeation Chromatography to Studies of Radical Scavenging by **Iodine**

L59 ANSWER 7 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Electrochemical oxidation of metal dialkyl phosphites and their reaction with halogens

L59 ANSWER 8 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Hydrogen iodide as dry etching gas for electronic devices and its manufacture

L59 ANSWER 9 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Preparation of spiro-piperidine derivatives and their use as therapeutic agents

L59 ANSWER 10 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Low-halogen polyalkylene-substituted carboxylic acylating agent compositions and compounds derived therefrom

L59 ANSWER 11 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Scavenger Assisted Trapping of Atomic Hydrogen in Si8O12-Cages

L59 ANSWER 12 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Heavy-Ion Radiolysis of Cyclooctane

L59 ANSWER 13 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Manufacture of propylene copolymers

L59 ANSWER 14 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Electrochemical synthesis of (.eta.5-cyclopentadienyl)cobalt-.eta.4-tetraphenylbutadienes and their interaction with **iodine**

L59 ANSWER 15 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI A convenient hydroiodination of olefins and alkynes with **hydrogen** iodide **generated** in situ

L59 ANSWER 16 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Preparation of ether-free [1.1.1]propellane and its telomers

L59 ANSWER 17 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Reactions of [1.1.1]propellane

L59 ANSWER 18 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI The radiation-induced formation of iodoalkanes and the radiolysis of iodomethane

L59 ANSWER 19 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Organorhodium(I) and -rhodium(III) complexes containing the ligand 1,1,1-tris[(diphenylphosphino)methyl]ethane (triphos)

L59 ANSWER 20 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Estrogen receptor binding affinity and uterotrophic activity of triphenylhaloethylenes

L59 ANSWER 21 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI vic-Iodo thiocyanates and iodo isothiocyanates. IX. A synthesis of penam and other polycyclic .beta.-lactams

L59 ANSWER 22 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Gaseous reagent generator

L59 ANSWER 23 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Synthesis and properties of bis(pentamethylcyclopentadienyl) actinide hydrocarbyls and hydrides. A new class of highly reactive f-element organometallic compounds

L59 ANSWER 24 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Application of allenylsilver(I) compounds in organic synthesis. A simple route to substituted allenes

L59 ANSWER 25 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Iodo-azide adducts of 3-methyl-.DELTA.2-steroids; structure and solvolysis

L59 ANSWER 26 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Characterization of hot chlorine atom reactions with hydrogen

L59 ANSWER 27 OF 27 HCA COPYRIGHT 2006 ACS on STN
TI Hydrogen iodide

```
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     FILE 'HCA' ENTERED AT 10:22:07 ON 26 APR 2006
L60         23282 S ((HYDROGEN# OR H2 OR H)(2A)(PRODUC? OR PROD# OR GENERAT
L61           297 S L60 AND L12
L62           279 S L61 NOT (L5/P OR L5/DP)
L63            23 S L62 AND (L8-L11 OR L42 OR HYDROCARBON#)
L64            18 S L63 NOT (L55-L58)
L65            16 S L64 NOT L59

=> d l65 1-16 ti
```

L65 ANSWER 1 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Solid phase oxidation of diene polymers with **hydrogen** peroxide and **formic** acid

L65 ANSWER 2 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Perspectives of a hydrogen energy economy Part 1: Techniques and systems for **hydrogen production**

L65 ANSWER 3 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Convenient, in Situ **Generation** of Anhydrous **Hydrogen** Iodide for the Preparation of .alpha.-Glycosyl Iodides and Vicinal Iodohydrins and for the Catalysis of Ferrier Glycosylation

L65 ANSWER 4 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Photochemical **hydrogen** iodide gas **generation** from iodomethane and 2-iodopropane

L65 ANSWER 5 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Studies on C-**H** activation. X. **Synthesis** of alkyl(carbonyl)hydrido- and allylhydridoosmium complexes by metal-initiated fragmentation of primary alcohols and olefins

L65 ANSWER 6 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Study of catalytic reduction of methanol for methane-methanol thermochemical **hydrogen production** cycles

L65 ANSWER 7 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Photochemical reactions. 139th Communication. Photochemistry of acylsilanes: 1. Siloxycarbene **formation** versus .gamma.-**hydrogen** abstraction

L65 ANSWER 8 OF 16 HCA COPYRIGHT 2006 ACS on STN

TI Regulation of proteophosphomannan biosynthesis in the scp yeast Candida maltosa **H** by precursor **preparation**

L65 ANSWER 9 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Liquid-phase carbon monoxide-**hydrogen** reactions: **synthesis** of acetaldehyde by homologation of methanol. II. Homologation in a chelating medium

L65 ANSWER 10 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Thermochemical **hydrogen preparation.** Part V. A feasibility study of the sulfur-**iodine** cycle

L65 ANSWER 11 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Reactions of photochemically **produced hydrogen** atoms at energies below 1.8 electron volts

L65 ANSWER 12 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI The isotope effect in the radiolytic **formation** of **hydrogen** from polyethylene

L65 ANSWER 13 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Chemical properties of high-energy **hydrogen** and carbon **produced** by nuclear reactions

L65 ANSWER 14 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Laboratory **preparation** of **hydrogen** sulfide from mixtures of sulfur and **hydrocarbons**

L65 ANSWER 15 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI A new effect of **hydrogen**-bond **formation.** V. Behavior of the 8-hydroxyl group in benzopyrone derivatives

L65 ANSWER 16 OF 16 HCA COPYRIGHT 2006 ACS on STN
TI Stereoisomerization of .alpha.-bromoallocinnamic acid and a preliminary observation on the addition **product** of **hydrogen** bromide and phenylpropiolic acid

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L65 ANSWER 2 OF 16 HCA COPYRIGHT 2006 ACS on STN
134:240008 Perspectives of a hydrogen energy economy Part 1: Techniques and systems for **hydrogen production.** Dreier, Thomas; Wagner, Ulrich (Energiewirtschaft und Anwendungstechnik an der TU Munchen, Germany). BWK: Brennstoff, Waerme, Kraft, 52(12), 41-46 (German) 2000. CODEN: BBWRAB. Publisher: Springer-VDI-Verlag GmbH & Co. KG.
AB In a review with 12 refs. the perspectives of a H2 energy economy

are outlined. The tech. systems to produce H2 are presented, starting with the steam reforming process of light **hydrocarbons** with water to achieve H2 and CO2. Other sources for H2 was the partial oxidn. of heavy residues from refineries, the gasification of coal, electrolysis of water, thermal decompn. of water, the sulfur-**iodine** process, solar-driven thermochem. processes, photosynthetic processes, and biol. processes.

CC 52-0 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 49

L65 ANSWER 6 OF 16 HCA COPYRIGHT 2006 ACS on STN
108:111749 Study of catalytic reduction of methanol for methane-methanol thermochemical **hydrogen production** cycles.
Onuki, K.; Shimizu, S.; Nakajima, H.; Ikezoe, Y.; Sato, S. (Japan At. Energy Res. Inst., Tokai, 319-11, Japan). International Journal of Hydrogen Energy, 12(8), 555-9 (English) 1987. CODEN: IJHEDX. ISSN: 0360-3199. OTHER SOURCES: CASREACT 108:111749.

AB MeOH was reduced to CH4 by HI in the presence of platinum ions. The reaction is considered to proceed sequentially from MeOH to MeI and then to CH4. Platinum ion acts as a catalyst for CH4 formation. In the presence of **iodine**, the reaction was greatly suppressed and the reaction rate was almost independent of temp. CH3-MeOH thermochem. H2 prodn. cycles utilizing the reaction are discussed.

IT **74-82-8P**, Methane, preparation
(prepn. of, by platinum-catalyzed redn. of methanol)
RN 74-82-8 HCA
CN Methane (8CI, 9CI) (CA INDEX NAME)

CH_4

CC 23-2 (Aliphatic Compounds)
IT **74-82-8P**, Methane, preparation
(prepn. of, by platinum-catalyzed redn. of methanol)

L65 ANSWER 10 OF 16 HCA COPYRIGHT 2006 ACS on STN
92:61074 Thermochemical **hydrogen preparation.** Part V. A feasibility study of the sulfur-**iodine** cycle.
Dokiya, M.; Kameyama, T.; Fukuda, K. (Natl. Chem. Lab. Ind., Tokyo, 153, Japan). International Journal of Hydrogen Energy, 4(4), 267-77 (English) 1979. CODEN: IJHEDX. ISSN: 0360-3199.

AB A S-I cycle consists of the following three reactions: 2H2O + SO2 + **I2** .fwdarw. H2SO4 + 2HI, H2SO4 .fwdarw. H2O + SO2 + 1/2O2, and 2HI .fwdarw. H2 + **I2.** The first reaction is performed as a cell reaction without the addn. of external energy, the H2SO4 and HI being produced sep. in the anode and cathode compartments,

resp. The 2nd and 3rd reactions are carried out as catalytic thermal decompns. A process flow sheet of this cycle and its mass balance was based on exptl. results, and the heat balance for this cycle was made. Internal heat exchange for this cycle is very large (.apprx.2600 kcal/mol H_2), mainly because of the low yield of the HI decompn. reaction. Theor. and exptl. studies were made to improve the yield of this reaction. The following three methods seem to be promising for this purpose: (1) continuous removal of the H produced in the reaction zone: (2) performance of the reaction at low temp. (185-250.degree.) and high pressure (100 atm); and (3) substitution of the benzene-**cyclohexane** cycle (6HI + **C_6H_6**
.fwdarw. **C_6H_{12}** + $3I_2$; **C_6H_{12}** .fwdarw.
C_6H_6 + $3H_2$) for the HI decompn. step.

IT **7553-56-2**, uses and miscellaneous
    (in hydrogen manuf., by cyclic thermochem. decompn. of water)

RN 7553-56-2 HCA

CN Iodine (8CI, 9CI) (CA INDEX NAME)

I— I

CC 49-1 (Industrial Inorganic Chemicals)
    Section cross-reference(s): 52

ST hydrogen cyclic thermochem manuf; water cyclic thermochem decompn; sulfur dioxide **iodine** cycle

IT 7732-18-5, reactions
    (decompn. of, by cyclic thermochem. process, **iodine** -sulfur cycle in)

IT 7446-09-5, uses and miscellaneous **7553-56-2**, uses and miscellaneous
    (in hydrogen manuf., by cyclic thermochem. decompn. of water)

IT 1333-74-0P, preparation
    (manuf. of, by cyclic thermochem. process, **iodine** -sulfur cycle in)